

ON A QUASI-MODULARITY PROPERTY OF THE POLYLOGARITHM GENERATING SERIES

SHELDON T JOYNER
THE UNIVERSITY OF WESTERN ONTARIO

ABSTRACT. A path space realization of $PSL(2, \mathbb{Z})$ is given, by means of which an action of this group on sections of the universal pronipotent bundle with connection on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ is produced. Under this action, the distinguished section given by the polylogarithm generating series $\text{Li}(z)$ is mapped to a family of formal power series each multiplied by $\text{Li}(z)$ itself. The resulting expressions are prototypical of statements of the quasi-modularity defined in the paper. In this case, the automorphy factors corresponding to the involutive and free generators of $PSL(2, \mathbb{Z})$ are respectively given by a transform of the DRINFEL'D associator and an R -matrix. Since we prove also that the associated mapping of $PSL(2, \mathbb{Z})$ into formal power series is injective, a power series realization of $PSL(2, \mathbb{Z})$ emerges which constitutes both an embedding of this group into the pronipotent completion of the fundamental group of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, and also into DRINFEL'D'S formal power series model of the quasi-triangular quasi-HOPF algebras. For certain qtqH algebras (satisfying an hypothesis on the R -matrix), a mapping of representations of such algebras into the representations of $PSL(2, \mathbb{Z})$ arises. The quasi-modularity provides an echo of usual modularity in an important example: RIEMANN'S contour integral proof of the functional equation of the zeta function $\zeta(s)$ is shown to belong to a family of proofs following from the quasi-modularity of $\text{Li}(z)$, reminiscent of the way in which the modularity of the theta function yields his FOURIER analysis proof.

CONTENTS

Introduction	2
Acknowledgements	5
1. Preliminaries	6
2. The reduced action on sections of \mathcal{U}	16
3. The path space realization of $PSL(2, \mathbb{Z})$	21
4. Quasi-modularity and the lifted action on sections of \mathcal{U}	30
5. The $PSL(2, \mathbb{Z})$ 1-cocycle on $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \mathbb{C})$	38
6. $PSL(2, \mathbb{Z})$ and the quasi-triangular quasi-HOPF algebras	39
7. Quasi-modularity in proving the functional equation of $\zeta(s)$	48
References	63

INTRODUCTION

Consider the monodromy representation χ of the fundamental group of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ which under the RIEMANN-HILBERT correspondence is associated to the universal pronipotent bundle \mathcal{U} with connection ∇ on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, (see [Hai94] for example). As is well known (cf. [Hai]), χ may be realized in $\mathbb{C} \langle\langle X_0, X_1 \rangle\rangle$, the ring of formal power series in non-commuting variables X_0 and X_1 with complex coefficients. This is done by associating CHEN series to the classes of paths in the fundamental group: Explicitly,

$$(1) \quad [\gamma] \mapsto \sum_w \int_{\gamma} \omega_{i_1} \dots \omega_{i_k} X_{i_1} \dots X_{i_k}$$

where the sum is taken over all words in the X_j (including the empty word, for which the corresponding integral is 1), and if z denotes the usual parameter on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, $\omega_0 = \frac{dz}{z}$ while $\omega_1 = \frac{dz}{1-z}$. (See [Hai].)

The main result of the present paper is the extension of the CHEN map of (1) to a 1-cocycle of $PSL(2, \mathbb{Z})$, into which the fundamental group embeds via the short exact sequence

$$(2) \quad 1 \rightarrow \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, c) \rightarrow PSL(2, \mathbb{Z}) \rightarrow SL(2, \mathbb{Z}/2\mathbb{Z}) \rightarrow 1,$$

(for any basepoint $c \in \mathbb{P}^1 \setminus \{0, 1, \infty\}$), arising from the universal covering of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ by the upper half plane - see §2.1 below.

The mapping which results is also the lift of a mapping of $SL(2, \mathbb{Z}/2\mathbb{Z})$ into $\mathbb{C} \langle\langle X_0, X_1 \rangle\rangle$ which may be deduced from work of OKUDA and UENO: In [OU05] the image of the polylogarithm generating series under an action of $SL(2, \mathbb{Z}/2\mathbb{Z})$ was computed. Power series arising from this action may be regarded as the images of the corresponding elements of $SL(2, \mathbb{Z}/2\mathbb{Z})$.

The map on $PSL(2, \mathbb{Z})$ is facilitated by an action of $SL(2, \mathbb{Z}/2\mathbb{Z})$ on the formal variables X_0 and X_1 arising from the formal KNIZHNIK-ZAMOLODCHIKOV equation $\nabla G = 0$, which was also given in [OU05]. Extending this action by linearity to the power series ring itself is a simple task. Write $\mathbb{C} \langle\langle X_0, X_1 \rangle\rangle_{\Lambda}^{\times}$ for $\mathbb{C} \langle\langle X_0, X_1 \rangle\rangle^{\times}$ equipped with this $SL(2, \mathbb{Z}/2\mathbb{Z})$ action.

Then one establishes the principal result of the paper, namely the

Theorem A. *The monodromy representation*

$$F_{\bullet} : \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \vec{01}) \rightarrow \mathbb{C} \langle\langle X_0, X_1 \rangle\rangle_{\Lambda}^{\times}$$

admits an extension to an injective 1-cocycle

$$F_{\bullet} : PSL(2, \mathbb{Z}) \rightarrow \mathbb{C} \langle\langle X_0, X_1 \rangle\rangle_{\Lambda}^{\times}.$$

(See 4.6, 4.8 and 4.11 below.)

Because of (2), the $SL(2, \mathbb{Z}/2\mathbb{Z})$ action is trivial on the image of the fundamental group, which is why $F_{\bullet}|_{\pi_1}$ is a homomorphism.

A key tool in the proof is the path space realization of $PSL(2, \mathbb{Z})$ with which §3 below is concerned. If $G_{\vec{ab}}$ denotes the set of homotopy classes of paths in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ emanating from \vec{ab} which end in any \vec{cd} with $a, b, c, d \in \{0, 1, \infty\}$ then we show

Theorem B. *For any \vec{ab} for which a and b are distinct elements of $\{0, 1, \infty\}$, $G_{\vec{ab}}$ may be endowed with a group operation by means of which it is isomorphic to $PSL(2, \mathbb{Z})$.*

(See 3.5 and 3.9 below.)

If $\Psi_{ab} : G_{\vec{ab}} \rightarrow PSL(2, \mathbb{Z})$ denotes the isomorphism, then the cocycle of Theorem A is given by:

$$\alpha \mapsto \sum_w \int_{\Psi^{-1}\alpha} \omega_{i_1} \dots \omega_{i_k} Y_{i_1} \dots Y_{i_k} \Big|_{Y_{i_j} = \bar{\alpha}^{-1} X_{i_j}},$$

with sum and ω_{i_j} notation as above, writing $\bar{\alpha}$ for the reduction of $\alpha \in PSL(2, \mathbb{Z})$ to $SL(2, \mathbb{Z}/2\mathbb{Z})$, and $\bar{\alpha}^{-1} X_{i_j}$ for the OKUDA-UENO action of $\bar{\alpha}^{-1} \in SL(2, \mathbb{Z}/2\mathbb{Z})$ on X_{i_j} .

The perspective adopted in much of the paper is that of actions of the respective groups on the sections of the prounipotent bundle \mathcal{U} . Framing Theorem A in these terms gives an action of $PSL(2, \mathbb{Z})$ on the polylogarithm generating series $\text{Li}(z, X_0, X_1)$. If ρ denotes the cyclic generator

$$\rho : \tau \mapsto 1 + \tau$$

of $PSL(2, \mathbb{Z})$ and

$$\sigma : \tau \mapsto -\frac{1}{\tau}$$

is the involutive generator, then we show

Theorem C.

$$(3) \quad \text{Li}^\rho(z, X_0, X_1) = e^{i\pi X_0} \text{Li}(z, X_0, X_1)$$

and

$$(4) \quad \text{Li}^\sigma(z, X_0, X_1) = \Phi_{KZ}(-X_1, -X_0) \text{Li}(z, X_0, X_1)$$

where Φ_{KZ} denotes the formal power series DRINFEL'D associator.

(See 4.7 below.)

Since the mapping

$$\rho \mapsto e^{i\pi X_0}; \quad \sigma \mapsto \Phi_{KZ}(-X_1, -X_0)$$

describes an injective $PSL(2, \mathbb{Z})$ 1-cocycle, the family of formal power series comprising the image of $PSL(2, \mathbb{Z})$ in $\mathbb{C} \ll X_0, X_1 \gg$ may be regarded as some kind of automorphy factor, whence the quasi-modularity of the polylogarithm generating series referred to in the title of the paper.

Together with Theorem A, this result also gives an easy way to compute the monodromy of the polylogarithms - see 4.10.

It is interesting that in the power series realization of $PSL(2, \mathbb{Z})$ given in Theorem A, σ corresponds to the DRINFEL'D associator while ρ corresponds to an R -matrix (in DRINFEL'D's formal power series model of the quasi-triangular quasi-HOPF algebras [henceforth qtqH algebras] given in [Dri91]). By means of this observation, we can prove that if $(A, \varepsilon, \Delta, R, \Phi)$ is a qtqH algebra in which

$$R = \sum a_i \otimes b_i = \sum b_i \otimes a_i$$

and

$$\Phi^{-1} = \left(\sum x_i \otimes y_i \otimes z_i \right)^{-1} = \sum z_i \otimes y_i \otimes x_i,$$

(which is always possible by means of some symmetric gauge transformation, see [Dri91]), then we have

Theorem D. *If R has $(\text{id} \otimes \Delta)R = (1 \otimes R)^{-1}$, then $PSL(2, \mathbb{Z})$ may be represented on $A \otimes A \otimes A$.*

Unless the representation factors through $SL(2, \mathbb{Z}/2\mathbb{Z})$, the induced functor from the category of representations $\text{Rep}A$ into $\text{Rep}PSL(2, \mathbb{Z})$ is not monoidal, since $\text{Rep}PSL(2, \mathbb{Z})$ is tannakian whereas $\text{Rep}A$ is quasi-tensored.

The power series realization of $PSL(2, \mathbb{Z})$ also has implications for the possible relations satisfied by the DRINFEL'D associator: Theorem A can be used to prove that if $E(X_0, X_1)$ is a formal power series, $E(X_0, X_1)^\alpha$ is the image of E under the action of $\bar{\alpha} \in SL(2, \mathbb{Z}/2\mathbb{Z})$ and \mathcal{E}_E denotes the space of sections

$$\{E(X_0, X_1)^\alpha F_\alpha(X_0, X_1) \text{Li}(z, X_0, X_1) | \alpha \in PSL(2, \mathbb{Z})\},$$

then

Theorem E. *For every $\bar{\eta} \in SL(2, \mathbb{Z}/2\mathbb{Z})$, $\mathcal{E}_{\Phi_{KZ}^{\bar{\eta}}}$ is a $PSL(2, \mathbb{Z})$ -torsor.*

Here, $\mathcal{E}_1 = \mathcal{E}_{\Phi_{KZ}^{\bar{\eta}}}$ but one can prove the

Theorem F. *$\mathcal{E}_{\Phi_{KZ}^{\bar{\eta}}}$ and \mathcal{E}_1 are disjoint whenever $\bar{\eta}$ is even as a permutation in S_3 .*

The quasi-modularity of the polylogarithm generating series parallels modularity of the JACOBI theta function $\theta(\tau)$ in the following sense: In the last section of the paper, a family of integral expressions for the RIEMANN zeta function $\zeta(s)$ is exhibited, arising from an additive iterativity property satisfied by iterated integrals. The theta function integral expression for $\zeta(s)$ is shown to belong to a complementary family coming from a multiplicative iterativity property. Now as HECKE established in [Hec36], analytic continuation and existence of the functional equation of $\zeta(s)$ are equivalent (modulo certain technical details) to the modularity of $\theta(\tau)$. By generalizing RIEMANN'S topological (contour integral) approach, using the members of the family of integrals coming from additive iterativity, we show that quasi-modularity of $\text{Li}(z, X_0, X_1)$ yields the proof of the analytic continuation and functional equation of $\zeta(s)$.

ACKNOWLEDGEMENTS

The author is glad of the chance to express his thanks to MINHYONG KIM for his unwavering encouragement and patient explanations, as well as for sharing his insights.

1. PRELIMINARIES

1.1. DELIGNE'S tangential basepoints and the fundamental path spaces. Suppose that $X = \overline{X} \setminus S$ is a smooth curve over \mathbb{C} where S is some finite set of points. In [Del89], DELIGNE introduced a notion of fundamental group of X based at any given omitted point $a \in S$, in the direction of some specified tangent vector to \overline{X} at a . Classically, as in [Hai94] such fundamental groups with *tangential basepoint* may be defined as follows: If $\vec{v}_j \in T_{a_j}$ is a tangent vector at $a_j \in S$ for $j = 0, 1$, set

$$P_{\vec{v}_0, \vec{v}_1} := \{\gamma : [0, 1] \rightarrow \overline{X} \mid \gamma'(0) = \vec{v}_0, \gamma'(1) = -\vec{v}_1, \gamma((0, 1)) \subset X\}.$$

Then

Definition 1.1. The fundamental path space $\pi_1(X, \vec{v}_0, \vec{v}_1)$ is the set of path components of $P_{\vec{v}_0, \vec{v}_1}$.

When $\vec{v}_1 = \vec{v}_0$, this is the fundamental group denoted $\pi_1(X, \vec{v}_0)$.

It is immediate that the fundamental path space $\pi_1(X, \vec{v}_0, \vec{v}_1)$ is a left $\pi_1(X, \vec{v}_0)$ -torsor and a right $\pi_1(X, \vec{v}_1)$ -torsor where the group actions are given by post- and pre-composition of paths of the respective fundamental groups by the classes of paths from \vec{v}_0 to \vec{v}_1 . The resulting isomorphisms are produced by the choice of a class of paths in $\pi_1(X, \vec{v}_0, \vec{v}_1)$, and hence are non-canonical.

On the other hand one can show that $\pi_1(X, \vec{v}_0)$ is naturally isomorphic to the usual topological fundamental group at any fixed point of X , cf. [Hai03].

This naive description is sufficient for the use of the paper. For our purposes, $\overline{X} = \mathbb{P}_{\mathbb{C}}^1$, $S = \{0, 1, \infty\}$, and \overrightarrow{ab} will denote the tangent vector of unit length over \overline{X} at $a \in S$, pointing in the direction of $b \in S$ for any $b \neq a$.

Definition 1.2. Any fundamental path space of the form of

$$\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{a_0 b_0}, \overrightarrow{a_1 b_1})$$

where $a_j, b_j \in \{0, 1, \infty\}$ and $a_j \neq b_j$ for $j = 0, 1$ will be called a *real-based fundamental path space* of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, and the tangential basepoints $\overrightarrow{a_j b_j}$ will be referred to as real tangential basepoints.

Fix a real tangential basepoint \overrightarrow{ab} . Then form the set

$$G_{\overrightarrow{ab}} := \cup \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{ab}, \overrightarrow{a_0 b_0})$$

where the union is taken over all $a_0, b_0 \in \{0, 1, \infty\}$ with $a_0 \neq b_0$. The utility of restricting attention to the real tangential basepoints lies in the fact that they admit an action of $SL(2, \mathbb{Z}/2\mathbb{Z})$, as will be discussed in §2. Using this action, $G_{\vec{ab}}$ will be endowed with a group structure in §3, by means of which it can be identified with $PSL(2, \mathbb{Z})$.

1.2. The universal prounipotent bundle with connection on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. For definitions and properties of CHEN iterated integrals, the reader is referred to [Hai] or [Joy10], and for general facts related to bundles with connections on curves (and parallel transport), to [Del70] or [Joy08]. Throughout, let X again denote some smooth curve over \mathbb{C} with $X = \overline{X} \setminus S$ for some finite set S . We begin by clarifying some terminology and stating certain facts without proof.

Definition 1.3. A bundle with connection (\mathcal{E}, ∇) on X is called *unipotent* whenever there exists a filtration by subbundles

$$\mathcal{E} = \mathcal{E}_0 \supset \mathcal{E}_1 \dots \supset \mathcal{E}_n \supset \mathcal{E}_{n+1} = 0$$

where each \mathcal{E}_i is stabilized by the connection

$$\nabla : \mathcal{E}_i \rightarrow \Omega_X^1 \otimes \mathcal{E}_i$$

and for each i ,

$$(\mathcal{E}_i / \mathcal{E}_{i+1}, \nabla) \xrightarrow{\sim} (\mathcal{O}_X^{r_i}, d)$$

for some integer r_i .

Denote the category of unipotent bundles with connection over X by $\mathbf{Un}(X)$.

The idea here is that unipotent connections are built up by extensions of successive connections, starting with the trivial connection; where an extension of connections is a short exact sequence

$$0 \rightarrow (\mathcal{E}_1, \nabla_1) \rightarrow (\mathcal{E}_2, \nabla_2) \rightarrow (\mathcal{E}_3, \nabla_3) \rightarrow 0$$

with the restriction of ∇_2 to \mathcal{E}_1 being ∇_1 and the quotient connection ∇_3 .

A bundle with connection (\mathcal{E}, ∇) on a manifold M is unipotent if and only if there exists a covering $\{U_\alpha\}$ of M and trivializations $\{e_{\alpha(1)}, \dots, e_{\alpha(k)}\}$ on U_α such that the connection matrices A_α are all strictly upper triangular. In the case of X as above, write $\{\kappa_1, \dots, \kappa_m\}$ for a basis for $H^1(X, \mathbb{C})$ (comprising algebraic differential forms on X). In more precise terms we have the well-known

Proposition 1.4. *If (\mathcal{E}, ∇) is a unipotent connection on such an X , then*

$$(\mathcal{E}, \nabla) \simeq (\mathcal{O}_X^r, d + \sum_{i=1}^m N_i \kappa_i)$$

where the N_i are constant matrices which are strictly upper triangular.

Refer to [Joy08] for the proof.

Example 1.5. Let $X = \mathbb{P}^1 \setminus \{0, 1, \infty\}$; $\mathcal{E} = \mathcal{O}_X^3$ and $\nabla = d + A$ with

$$A = \begin{pmatrix} 0 & -\frac{dz}{z} & 0 \\ 0 & 0 & -\frac{dz}{1-z} \\ 0 & 0 & 0 \end{pmatrix}.$$

Then

$$\tilde{f} := \begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix}$$

is flat if and only if

$$d\tilde{f} = -A\tilde{f}$$

-i.e. $df_3 = 0$; $df_2 = f_3 \frac{dz}{1-z}$ and $df_1 = f_2 \frac{dz}{z}$. The solution to this system is given by

$$\begin{aligned} f_3 &= a; \quad f_2 = a \int \frac{dz}{1-z} + b \\ f_1 &= a \int \frac{dz}{1-z} \frac{dz}{z} + b \int \frac{dz}{z} + c \end{aligned}$$

where a, b and c are some constants and the first integral in the expression for f_1 is iterated in the sense of CHEN (see [Hai]). Therefore, along any path γ , if

$$P(\gamma) := \begin{pmatrix} 1 & \int_{\gamma} \frac{dz}{z} & \int_{\gamma} \frac{dz}{1-z} \frac{dz}{z} \\ 0 & 1 & \int_{\gamma} \frac{dz}{1-z} \\ 0 & 0 & 1 \end{pmatrix}$$

then $P(\gamma)v$ is the value of a flat section of $\mathcal{E}_{\gamma(1)}$ for any $v = (c \ b \ a)^T \in \mathcal{E}_{\gamma(0)}$, determined along γ .

It is evident from the proposition that this bundle with connection is unipotent, but this may also be shown by a direct calculation which is left to the reader.

Over $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, the unipotent bundles of the form typified by the above example are natural objects of study. The fundamental object we proceed to construct is a subbundle of the inverse limit of such bundles:

The construction is given in the context of more general X , and we begin by forming an inverse limit of unipotent bundles which satisfies a universal property with respect to the objects of $\mathbf{Un}(X)$. To this end, define $\mathbb{C} \langle A_1, \dots, A_m \rangle$ to be the free associative algebra of polynomials in the non-commuting variables A_1, \dots, A_m , with augmentation ideal $I := (A_1, \dots, A_m)$. Then let

$$U_n := \mathbb{C} \langle A_1, \dots, A_m \rangle / I^{n+1},$$

i.e. the algebra comprising linear combinations of words in the A_j of length less than or equal to n . The inverse limit of the U_n is the power series algebra in the non-commuting variables

$$U := \varprojlim U_n = \mathbb{C} \langle\langle A_1, \dots, A_m \rangle\rangle.$$

Now we set $\mathcal{U}_n := U_n \otimes \mathcal{O}_X$ and $\mathcal{U} := \varprojlim \mathcal{U}_n$. With the κ_j defined as above for $j = 1, \dots, m$, and $|w|$ denoting the length of the word w in the A_j , a compatible family of connections on the \mathcal{U}_n can be defined, giving rise to a connection on \mathcal{U} : Indeed, let

$$\sum_{|w| \leq n} f_w[w] \in \mathcal{U}_n$$

be arbitrary, and set

$$\nabla_n \left(\sum_{|w| \leq n} f_w[w] \right) = \sum_{|w| \leq n} df_w[w] - pr_n \sum_{|w| \leq n} f_w \sum_{i=1}^m \kappa_i[wA_i]$$

where pr_n is the projection to \mathcal{U}_n - i.e. the augmented words $[wA_i]$ having length greater than n are disregarded. Then ∇_n is a connection on \mathcal{U}_n , from the usual LEIBNITZ rule $d(ff_w) = (df)f_w + fdf_w$ on \mathcal{O}_X . Moreover, for $k > 0$, the (suitably interpreted) restriction of the connection on \mathcal{U}_{n+k} to \mathcal{U}_n evidently agrees with ∇_n . These connections are all unipotent because each algebra \mathcal{U}_n is isomorphic to $\mathcal{O}_X^{k_n}$ where k_n is the number of words in the A_j of length less than or equal to n ; and the connections are all of the form $d + \sum_{i=1}^m M_i \kappa_i$ where each M_i is strictly upper triangular by virtue of the lengthening of words by A_i in the formula.

Hence (\mathcal{U}, ∇) is the inverse limit of unipotent connections on X . It is universal in the following sense:

Proposition 1.6. *Let $b \in X$ and denote by (\mathcal{E}, ∇') any fixed unipotent connection on X . Suppose that $v \in \mathcal{E}_b$. Then there exists a unique morphism*

$$\phi_v : (\mathcal{U}, \nabla) \rightarrow (\mathcal{E}, \nabla')$$

in the category of bundles with connection over X , such that

$$(\phi_v)_b(1) = v.$$

This proposition is the topological version of an analogous result proven by MINHYONG KIM in [Kim09], and the proof here is also due to him. Certain constructions in the proof will be useful in what follows, so we include it:

Proof. Recall that $(\mathcal{E}, \nabla') \xrightarrow{\sim} (\mathcal{O}_X^r, d - \sum_{i=1}^m N_i \kappa_i)$ for some positive integer r and suitable N_i . If $k_{n-1} < r \leq k_n$ where there are k_n words of length less than or equal to n , it suffices to define the mapping of \mathcal{U} to \mathcal{E} via \mathcal{U}_n . Now given a word $w = A_{i_1} \dots A_{i_k}$, let $N_w = N_{i_1} \dots N_{i_k}$ and define

$$\phi : \sum_{|w| \leq n} f_w[w] \mapsto \sum_{|w| \leq n} f_w N_w v.$$

This gives a mapping of \mathcal{U} to \mathcal{E} which is compatible with the connections, as an easy calculation shows. (One sees that $\phi \circ \nabla = \nabla' \circ \phi$.)

To show the uniqueness, it suffices to demonstrate that ϕ_v is determined by $(\phi_v)_b(1)$ and the compatibility with ∇ .

Firstly we remark that the mapping on fibers above b induced by ϕ , namely $\phi_b : \mathcal{U}_b \rightarrow \mathcal{E}_b$, is compatible with the action of $\pi_1(X, b)$ via parallel transport. The reason for this is that each bundle with connection determines a π_1 representation, so by compatibility with ∇ , ϕ_b is a map of π_1 representations. Hence for any $y \in \mathcal{U}_b$, and any $\gamma \in \pi_1(X, b)$,

$$\phi_b(\gamma \cdot y) = \gamma \cdot \phi_b(y),$$

where the latter denotes the parallel transport action of γ on the element $\phi_b(y)$ of \mathcal{E}_b .

It thus remains to show that $\mathbb{C}[\pi_1] \cdot 1 = (\mathcal{U}_n)_b$ where $1 \in \mathcal{U}_n$ - i.e. the action of the group algebra $\mathbb{C}[\pi_1]$ on 1 generates all of $(\mathcal{U}_n)_b$.

To demonstrate this, we give a concrete description of parallel transport in \mathcal{U} . This is achieved by means of a specific global flat section: Let

$$(5) \quad G(z) := \sum_w \int_c^z \kappa_w[w]$$

for some fixed $c \in X$, with $\kappa_w = \kappa_{i_1} \dots \kappa_{i_k}$ if $w = A_{i_1} \dots A_{i_k}$ and the integrals are iterated along a path from c to z which does not loop about any of the points of S . G is a sort of generating function of the homotopy functionals determined by the iterated integrals, and is usually referred to as a CHEN series. It is also a flat section of

the bundle \mathcal{U} : Recall that if $F(z) := \int_c^z \beta_1 \beta_2 \dots \beta_r$, then $dF(z) = \beta_r \cdot \int \beta_1 \dots \beta_{r-1}$. Therefore

$$dG = \sum_{i=1}^m \kappa_i \sum_w \int_c^z \kappa_w [w A_i]$$

and consequently,

$$(6) \quad \nabla(G) = 0.$$

Now using the geometric description of parallel transport along a given path γ , consider the unique flat section s satisfying $s(b) = 1$. Taking $c = b$ in the definition of G , this flat section is the same as G , since if $I_b \in \pi_1(X, b)$ denotes the trivial path,

$$\sum_w \int_{I_b} \kappa_w [w] = \sum_w 0[w] = \text{the empty word} = 1.$$

But G is defined along the lift of any $\gamma \in \pi_1(X, b)$, so for such a path,

$$P(\gamma)(1) = \sum_w \int_\gamma \kappa_w [w] =: \gamma \cdot 1,$$

giving the parallel transport along γ of the element $1 \in \mathcal{U}_b$. This action extends to an action of the group algebra $\mathbb{C}[\pi_1]$ in a natural way: For $\gamma = \sum_i c_i \gamma_i$, take

$$\int_\gamma \kappa_w := \sum_i c_i \int_{\gamma_i} \kappa_w.$$

The mapping thereby induced, of $\mathbb{C}[\pi_1]$ into $(\mathcal{U}_n)_b$ via $\gamma \mapsto \gamma \cdot 1$ is a surjection. Were this not the case, then $\mathbb{C}[\pi_1]$ would map into a linear subspace, for which $\sum_w c_w \int_\gamma \kappa_w = 0$ for all $\gamma \in \mathbb{C}[\pi_1]$.

To conclude the proof, it thus suffices to show that the iterated integrals $\int \kappa_w$ are linearly independent as functions on $\mathbb{C}[\pi_1]$.

Consider a dual basis for $H_1(X, \mathbb{C})$ to the κ_j , say $\{[\mu_1], \dots, [\mu_m]\}$ and lift these to representatives $\mu_j \in \mathbb{C}[\pi_1]$. (Recall that

$$\mathbb{C}[\pi_1] \rightarrow \mathbb{C}[\pi_1/[\pi_1, \pi_1]] \rightarrow H_1(X, \mathbb{C}).)$$

The linear independence may now be shown by induction on word length: Certainly it is true for the empty word, so assume that it is known to be true for all words of length less than or equal to some k . If, however,

$$(7) \quad \sum_{|w| \leq k+1} c_w \int_\gamma \kappa_w = 0$$

holds for *all* $\gamma \in \mathbb{C}[\pi_1]$, then we can rewrite this equation using any fixed μ_j as follows:

$$\begin{aligned}
0 &= \sum_i \sum_{|w| \leq k} c_{A_i w} \int_{\mu_j \gamma} \kappa_{A_i w} \\
&= \sum_i \sum_{|w| \leq k} c_{A_i w} \left(\int_{\gamma} \kappa_{A_i w} + \int_{\mu_j} \kappa_i \int_{\gamma} \kappa_w + \text{other terms} \right) \quad \text{by coproduct} \\
&= \sum_i \sum_{|w| \leq k} c_{A_i w} \int_{\gamma} \kappa_{A_i w} + \sum_i \sum_{|w|=k} c_{A_i w} \delta_{ji} \int_{\gamma} \kappa_w + \sum_{|w| < k} c' \int_{\gamma} \kappa_w \\
&= 0 + \sum_{|w|=k} c_{A_j w} \int_{\gamma} \kappa_w + \sum_{|w| < k} c' \int_{\gamma} \kappa_w \quad \text{by (7)}.
\end{aligned}$$

By the induction hypothesis, the $c_{A_j w}$ are all zero, and this holds for all j . Hence, again by the induction, all of the other coefficients of the expression in (7) are zero too. \square

Next we recall some algebraic constructions which provide motivation for the definition of a fundamental object of study in this paper. If H is a discrete group and Q a ring, denote the group ring by $Q[H]$ and the augmentation ideal by J . The latter is the kernel of the mapping $\varepsilon : Q[H] \rightarrow Q$ defined by

$$\varepsilon : \sum_{h \in H} c_h h \mapsto \sum_{h \in H} c_h.$$

The pronipotent completion of H over Q consists of the group-like elements of the J -adic completion of the group ring $Q[H]$ which are congruent to 1 modulo J . Here the coproduct is defined on the completion by extending the coproduct under which the elements h of H have $\Delta h = h \otimes h$. It is possible to show that the group-like elements coincide with the (formal) exponentials of the elements of the completion of the free LIE algebra over the generators of H with Q coefficients - the so-called LIE exponentials, cf. [Reu93].

Bearing this in mind, notice that each ring U_n may be endowed with a coproduct by \mathbb{C} -linearly extending the coproduct under which the A_j are primitive (i.e. $\Delta A_j = A_j \otimes 1 + 1 \otimes A_j$). This induces a coproduct $\hat{\otimes}$ on the inverse limit of the U_n . As above, the *group-like* elements of U are those formal power series $F(A_1, \dots, A_m)$ for which $\Delta F = F \hat{\otimes} F$. The group-like elements which are congruent to 1 modulo I form the group of LIE exponentials.

Define $Ch(\mathcal{U})$ to be the space of sections of \mathcal{U} which like the CHEN series have local expressions of the form of

$$\sum_w f_w(z)[w] = \sum_w \sum_{j=1}^{n_w} a_j^w \int_{\gamma_j} f_j^w(\kappa_1, \dots, \kappa_m)[w]$$

at $z \in X$, where the a_j^w are elements of \mathbb{C} , $\gamma_j \in \pi_1(X, c, z)$ are (homotopy classes of) paths in X between the points c and z in X , and the f_j^w are monomial expressions in the κ_j so that the integrals are understood to be iterated over these expressions. By CHEN's π_1 DERHAM Theorem (see [Hai]), $Ch(\mathcal{U})$ is obtained by replacing \mathcal{O}_X in the construction of \mathcal{U} with the space of homotopy functionals on X with respect to some fixed basepoint $c \in X$. Then $Ch(\mathcal{U})$ may also be endowed with a coproduct, inherited from the comultiplication formula for iterated integrals (ibid.) while extending the coproduct on U . It is possible to show that $G(z) \in \Gamma(V_z, Ch(\mathcal{U}))$ is group-like with respect to this comultiplication.

By concatenation of paths, $Ch(\mathcal{U})_z$ is equipped with a right action of the prounipotent completion $\pi_1^{\text{un}}(X, z)$ of $\pi_1(X, z)$ (i.e. the group-like elements of the inverse limit over the quotients

$$\mathbb{C}[\pi_1(X, z)]/J_{\pi_1}^n$$

where J_{π_1} denotes the augmentation ideal). $Ch(\mathcal{U})$ also comes with a left action of $\pi_1^{\text{un}}(X, c)$, and similar to the version of parallel transport presented in the proof of the theorem, the prounipotent completion of $\pi_1(X, z, y)$ acts on $Ch(\mathcal{U})_z$ on the right, sending it onto $Ch(\mathcal{U})_y$.

These actions respect the space \mathcal{P} of group-like sections of $Ch(\mathcal{U})$, and are faithful transitive actions. Most notably, \mathcal{P} is a right $\pi_1^{\text{un}}(X, c)$ -torsor over X , which in line with the analogous notions in [Kim09] we refer to henceforth as the *canonical torsor*. Notice that the connection on \mathcal{U} restricts to \mathcal{P} .

In the particular case of interest, taking $X = \mathbb{P}^1 \setminus \{0, 1, \infty\}$, the equation (6) satisfied by flat sections is known as the formal KNIZHNIK-ZAMOLODCHIKOV equation [Dri91], explicitly (with $A_1 = X_0$, $A_2 = X_1$ and $m = 2$),

$$\left[d - \frac{dz}{z} X_0 - \frac{dz}{1-z} X_1 \right] G(z) = 0.$$

Then in the construction of a solution by (5), take $b = \overrightarrow{01}$ and let γ denote the path from $\overrightarrow{01}$ to any z in X (other than points of the real axis greater than 1 or less than 0), which does not cross the real axis unless $z \in (0, 1)$, in which case the path lies along the real axis. Then

the corresponding flat section of (5) is known as the polylogarithm generating function $\text{Li}(z, X_0, X_1)$. Moreover, the suitably regularized parallel transport action $P((0, 1)) \cdot 1$ gives the DRINFEL'D associator $\Phi_{KZ}(X_0, X_1)$ (cf. [Car01] for the regularization). Both $\text{Li}(z, X_0, X_1)$ and $\Phi_{KZ}(X_0, X_1)$ are known to be group-like (ibid.).

Writing $\kappa_0 = \frac{dz}{z}$ and $\kappa_1 = \frac{dz}{1-z}$, in notation of the proof of the Theorem,

$$\text{Li}(z, X_0, X_1) = \sum_w \int_\gamma \kappa_w[w]$$

where the $[w]$ run over all words in the non-commuting formal variables X_0 and X_1 . When κ_w is of the form of

$$\frac{dz}{1-z} \left(\frac{dz}{z} \right)^{k_1-1} \frac{dz}{1-z} \left(\frac{dz}{z} \right)^{k_2-1} \cdots \frac{dz}{1-z} \left(\frac{dz}{z} \right)^{k_r-1},$$

then

$$\int_\gamma \kappa_w = \sum_{0 < m_1 < \dots < m_r} \frac{z^{m_r}}{m_1^{k_1} \dots m_r^{k_r}},$$

the multiple polylogarithm function, [Car01].

It is not hard (see [MPvdH00] or [Car01]) to establish the asymptotics

$$(8) \quad Li(\varepsilon) = \exp(X_0 \log \varepsilon) + O(\sqrt{\varepsilon})$$

as $\varepsilon \rightarrow 0^+$ with $\varepsilon \in \mathbb{R}$. Effectively,

$$\lim_{z \rightarrow 0} \exp(-X_0 \log z) \text{Li}(z, X_0, X_1) = \lim_{z \rightarrow 0} \text{Li}(z, X_0, X_1) \exp(-X_0 \log z) = 1$$

entails regularization of $\text{Li}(z, X_0, X_1)$ at $z = 0$, and characterizes this series among solutions to (6).

At the same time, as in [Car01], one can show that $\Phi_{KZ}(X_0, X_1)$ admits of concrete description in terms of regularizations of polylogarithm generating series, by means of which it is possible to show

$$\lim_{z \rightarrow 1} \text{Li}(z, X_0, X_1) \exp(X_1 \log(1-z)) = \Phi_{KZ}(X_0, X_1).$$

1.3. The DELIGNE canonical extension and the canonical base-point. In [Del70], DELIGNE gave a canonical means of extending a given bundle \mathcal{E}' with flat connection $\tilde{\nabla}'$ defined over the punctured disc D' , to a holomorphic bundle (say \mathcal{E}) with connection (say $\tilde{\nabla}$) over the disc D . $(\mathcal{E}, \tilde{\nabla})$ is characterised as being the unique extension of $(\mathcal{E}', \tilde{\nabla}')$ for which the connection has a regular singular point at the origin with nilpotent residue. Again we are following HAIN'S presentation in [Hai03] to introduce the notion only in the setting in which it is required here. (For greater generality cf. [Del70].)

Let $\{\phi_1(z), \dots, \phi_m(z)\}$ denote an ordered basis of flat local sections of \mathcal{E}' near some point of D' . Around the origin, such sections are typically multi-valued, and the trick is to destroy the monodromy. This is done as follows: Let T denote the monodromy operator about the origin, and set

$$N := \frac{1}{2\pi i} \log T.$$

Then for $j = 1, \dots, m$ define

$$\psi_j(z) := z^{-N} \phi_j(z).$$

The monodromy of $z^{-N} = \exp(-N \log z)$ about 0 is $\exp(-N 2\pi i) = T^{-1}$ whereas $\phi_j(z)$ continued analytically about 0 is $T\phi_j(z)$, so one sees that $\psi_j(z)$ is single-valued on D for every j . The $\psi_j(z)$ give a framing for the DELIGNE canonical extension of \mathcal{E} to D , and

$$\tilde{\nabla} := d - N \frac{dz}{z}.$$

If X is some RIEMANN surface with compactification \overline{X} such that $S = \overline{X} \setminus X$ is finite, the local construction of the canonical extension may be given at each of the points of S and then glued to yield an extension of a given flat bundle over X to a holomorphic bundle over \overline{X} , in a canonical way. As before, the extension is referred to as the DELIGNE canonical extension.

The following construction is also due to DELIGNE: With X and \overline{X} as above, the fibre functor from $\mathbf{Un}(X)$ into $\mathbf{Vect}(\overline{X})$ given by associating to any object of $\mathbf{Un}(X)$ the global sections of the DELIGNE canonical extension to \overline{X} is referred to as the canonical basepoint. The reason for this terminology is that in the pattern of GROTHENDIECK's arithmetic fundamental groups, one can define the unipotent completion $\pi_1^{\text{un}}(X, \mathcal{C})$ of the fundamental group at the canonical basepoint as the group of tensor-compatible automorphisms of \mathcal{C} .

1.4. Quasi-triangular quasi-HOPF algebras. An algebra A over a commutative ring k is called quasi-triangular quasi-HOPF (henceforth qtqH) if it is equipped with a counit ε and comultiplication Δ with respect to which both cocommutativity and coassociativity fail in a controlled way. More precisely, a qtqH algebra is a k -algebra A such that the category $\text{Rep} A$ of representations of A is a braided monoidal (otherwise called quasi-tensored) category, where the natural isomorphisms governing the failure of commutativity and associativity of the quasi-tensor product functor correspond to distinguished elements R of $A \otimes A$ and Φ of $A \otimes A \otimes A$ respectively. Any such R is known as

an R -matrix and furnishes a solution to the YANG-BAXTER equation, while Φ is referred to as the DRINFEL'D associator and is unique up to certain gauge transformations. See [Dri91] for the details.

Strictly speaking, one refers to $(A, \varepsilon, \Delta, \Phi, R)$ as the qtqH algebra, but often (as above) we abuse this usage and refer to A as the qtqH algebra.

For later use, we record the hexagonal relations which dictate how given R and Φ interact: Write $\tilde{R} = 1 \otimes R$. Then if $Z \in A \otimes A \otimes A$ is of the form of $\sum x_i^1 \otimes x_i^2 \otimes x_i^3$, for any permutation δ of the indices 1, 2, and 3, we write $Z^{\delta(1)\delta(2)\delta(3)}$ to denote $\sum x_i^{\delta^{-1}(1)} \otimes x_i^{\delta^{-1}(2)} \otimes x_i^{\delta^{-1}(3)}$. Then one has

$$(9) \quad (\Delta \otimes id)R = \Phi^{312} \tilde{R}^{213} (\Phi^{132})^{-1} \tilde{R} \Phi$$

and

$$(10) \quad (id \otimes \Delta)R = (\Phi^{231})^{-1} \tilde{R}^{213} \Phi^{213} R^{312} \Phi^{-1}.$$

The corresponding equalities of natural transformations of the quasi-tensor give the so-called braiding in $\text{Rep}A$.

2. THE REDUCED ACTION ON SECTIONS OF \mathcal{U}

1. The group of Deck transformations of the covering of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ by the upper half plane \mathcal{H} is known to be given by the congruence subgroup

$$\begin{aligned} \Gamma(2)/\{\pm I\} &:= \left\{ \tau \mapsto \frac{a\tau + b}{c\tau + d} \in PSL(2, \mathbb{Z}) \mid \begin{bmatrix} a & b \\ c & d \end{bmatrix} \equiv \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \text{ modulo } 2 \right\} \\ &= \langle \tau \mapsto \tau + 2, \tau \mapsto \frac{\tau}{1 - 2\tau} \rangle. \end{aligned}$$

(See [Cha80] for example.) As the kernel of the surjection $PSL(2, \mathbb{Z}) \rightarrow SL(2, \mathbb{Z}/2\mathbb{Z})$, $\Gamma(2)/\{\pm I\}$ is a normal subgroup and we have the short exact sequence

$$(11) \quad 1 \rightarrow \Gamma(2)/\{\pm I\} \rightarrow PSL(2, \mathbb{Z}) \rightarrow SL(2, \mathbb{Z}/2\mathbb{Z}) \rightarrow 1.$$

Since \mathcal{H} is the universal covering space of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, in fact

$$\Gamma(2)/\{\pm I\} \simeq \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, x),$$

the topological fundamental group of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ at any chosen base-point $x \in \mathbb{P}^1 \setminus \{0, 1, \infty\}$. As mentioned before, it is known (cf. [Hai03]) that

$$\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, x) \simeq \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \vec{ab})$$

for any real tangential basepoint \overrightarrow{ab} . Thus, (11) becomes

$$(12) \quad 1 \rightarrow \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{01}) \rightarrow PSL(2, \mathbb{Z}) \xrightarrow{A} SL(2, \mathbb{Z}/2\mathbb{Z}) \rightarrow 1$$

which has an important role to play below.

2. Again from [Cha80], the function

$$\lambda(\tau) = \frac{\{\sum_{n \in \mathbb{Z}} \exp[i\pi\tau(n + 1/2)^2]\}^4}{\{\sum_{n \in \mathbb{Z}} \exp[i\pi\tau n^2]\}^4}$$

is known to effect the covering $\mathcal{H} \rightarrow \mathbb{P}^1 \setminus \{0, 1, \infty\}$. For this to be the case, $\lambda(\tau)$ is necessarily modular with respect to $\Gamma(2)$. At the same time, $\lambda(\tau)$ exhibits certain symmetries under the action of the respective cosets of $\Gamma(2)/\{\pm I\}$ in $PSL(2, \mathbb{Z})$ - that is to say, under an action of $SL(2, \mathbb{Z}/2\mathbb{Z})$. As is described in [Cha80], these symmetries are captured by the classical anharmonic group Λ , to which $SL(2, \mathbb{Z}/2\mathbb{Z})$ is thus isomorphic. Λ is given explicitly as the following group of linear fractional automorphisms of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$:

$$\Lambda = \left\{ \lambda \mapsto \lambda, \lambda \mapsto 1 - \lambda, \lambda \mapsto \frac{\lambda}{\lambda - 1}, \lambda \mapsto \frac{1}{\lambda}, \lambda \mapsto \frac{\lambda - 1}{\lambda}, \lambda \mapsto \frac{1}{1 - \lambda} \right\}.$$

It is evident from the topology that Λ is exactly the group of *all* such linear fractional automorphisms of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$.

Note that these transformations necessarily permute the real tangential basepoints, as is also immediate from the above explicit description. In fact, the elements of Λ are characterized by the corresponding permutations of the symbols 0, 1 and ∞ : We have

Lemma 2.1.

$$\Lambda \simeq S_3$$

Proof. The proof is elementary, for example identifying $(\lambda \mapsto 1 - \lambda)$ with the transposition (01), and $(\lambda \mapsto \frac{\lambda}{\lambda - 1})$ with (1 ∞). \square

Once and for all fix isomorphisms

$$(13) \quad SL(2, \mathbb{Z}/2\mathbb{Z}) \simeq \Lambda \simeq S_3 \simeq \langle \bar{\sigma}, \bar{\rho} | \bar{\sigma}^2 = \bar{\rho}^2 = 1; \bar{\sigma}\bar{\rho}\bar{\sigma} = \bar{\rho}\bar{\sigma}\bar{\rho} \rangle$$

by identifying the respective generators

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \leftrightarrow (\lambda \mapsto 1 - \lambda) \leftrightarrow (01) \leftrightarrow \bar{\sigma}$$

and

$$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \leftrightarrow (\lambda \mapsto \frac{\lambda}{\lambda - 1}) \leftrightarrow (1\infty) \leftrightarrow \bar{\rho}.$$

3. The Λ action on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ by linear fractional transformations lifts to the (global) sections of $\mathcal{O}_{\mathbb{P}^1 \setminus \{0, 1, \infty\}}$ in the obvious way. This produces an action on sections of \mathcal{U} once a suitable action of Λ on the formal variables X_0 and X_1 is defined. The latter was determined by OKUDA and UENO in [OU05], in which formal algebraic arguments and the theory of differential equations was used to compute the Λ action on the fundamental solutions to the KZ equation with specific asymptotics at 0, 1 and ∞ respectively, generalizing a calculation of DRINFEL'D. The action on X_0 and X_1 arises from a simple substitution action on the KZ equation:

Example 2.2. Consider the element $\bar{\sigma} : z \mapsto 1 - z$ of Λ . Making this substitution in the KZ equation yields

$$-\frac{d}{dz}G(1-z, X_0, X_1) = \left(\frac{X_0}{1-z} + \frac{X_1}{z} \right) G(1-z, X_0, X_1)$$

- i.e.

$$(14) \quad \frac{d}{dz}\tilde{G}(z, X_0, X_1) = \left(\frac{-X_1}{z} + \frac{-X_0}{1-z} \right) \tilde{G}(z, X_0, X_1).$$

This equation is identical to the original KZ equation but for the interchanging of $X_0 \leftrightarrow -X_1$. Therefore we define the action of $\bar{\sigma}$ on the pair (X_0, X_1) of formal non-commuting variables introduced in §1.2, as the involution $(X_0, X_1) \mapsto (-X_1, -X_0)$.

This example may be imitated for each element of Λ , and as in [OU05] it is convenient to summarize all transformations of (X_0, X_1) which arise in this way. The associated linear fractional transformations of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ are also tabulated:

Elt. of $SL(2, \mathbb{Z}/2\mathbb{Z})$	Lin. frac. tr.	Action on (X_0, X_1)
1	$z \mapsto z$	$(X_0, X_1) \mapsto (X_0, X_1)$
$\bar{\sigma}$	$z \mapsto 1 - z$	$(X_0, X_1) \mapsto (-X_1, -X_0)$
$\bar{\rho}$	$z \mapsto \frac{z}{z-1}$	$(X_0, X_1) \mapsto (X_0, X_0 - X_1)$
$\bar{\sigma} \circ \bar{\rho}$	$z \mapsto \frac{1}{1-z}$	$(X_0, X_1) \mapsto (X_1 - X_0, -X_0)$
$\bar{\rho} \circ \bar{\sigma}$	$z \mapsto \frac{z-1}{z}$	$(X_0, X_1) \mapsto (-X_1, X_0 - X_1)$
$\bar{\rho} \circ \bar{\sigma} \circ \bar{\rho} = \bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma}$	$z \mapsto \frac{1}{z}$	$(X_0, X_1) \mapsto (X_1 - X_0, X_1)$

Now one can state the

Definition 2.3. For every $\bar{v} \in SL(2, \mathbb{Z}/2\mathbb{Z})$ and every global section $L(z, X_0, X_1)$ of \mathcal{U} , set

$$L^{\bar{v}}(z, X_0, X_1) := L(\bar{v}(z), \bar{v}^{-1}X_0, \bar{v}^{-1}X_1)$$

and refer to this as the $SL(2, \mathbb{Z}/2\mathbb{Z})$ -action on global sections of \mathcal{U} .

Example 2.4. We compute $\text{Li}^{\bar{\sigma}}(z, X_0, X_1)$: By construction,

$$\text{Li}^{\bar{\sigma}}(z, \bar{\sigma}X_0, \bar{\sigma}X_1) = \text{Li}(1 - z, X_0, X_1)$$

is a fundamental solution to (14). Formally, $\text{Li}(z, -X_1, -X_0)$ is also. Recall from §1.2 that

$$\text{Li}(z, X_0, X_1) \exp(-X_0 \log z) \rightarrow 1$$

as $z \rightarrow 0$. Hence

$$(15) \quad \text{Li}(z, -X_1, -X_0) \exp(X_1 \log z) \rightarrow 1$$

as $z \rightarrow 0$. Now recall

$$\lim_{z \rightarrow 1} \text{Li}(z, X_0, X_1) \exp(X_1 \log(1 - z)) = \Phi_{KZ}(X_0, X_1),$$

or equivalently,

$$\lim_{z \rightarrow 0} \text{Li}(1 - z, X_0, X_1) \exp(X_1 \log z) = \Phi_{KZ}(X_0, X_1).$$

But then $\Phi_{KZ}(X_0, X_1)\text{Li}(z, -X_1, -X_0)$ and $\text{Li}(1 - z, X_0, X_1)$ share the same asymptotics near zero and both are solutions to the KZ equation. By uniqueness of such solutions, then

$$\text{Li}^{\bar{\sigma}}(z, X_0, X_1) = \text{Li}(1 - z, -X_1, -X_0) = \Phi_{KZ}(-X_1, -X_0)\text{Li}(z, X_0, X_1)$$

We remark that by the symmetry in the above computation, it is evident that $\Phi_{KZ}(X_0, X_1)^{-1} = \Phi_{KZ}(-X_1, -X_0)$, a fact which will be used often in what follows.

With the notation of 2.3, the computations of [OU05], (which run in the same vein as 2.4), may be summarized by

Proposition 2.5.

$$\begin{aligned} \text{Li}^{\bar{\sigma}}(z, X_0, X_1) &= \Phi_{KZ}(-X_1, -X_0)\text{Li}(z, X_0, X_1) \\ \text{Li}^{\bar{\rho}}(z, X_0, X_1) &= \exp(\mp X_0 i\pi)\text{Li}(z, X_0, X_1) \\ \text{Li}^{\bar{\sigma}\bar{\rho}}(z, X_0, X_1) &= \exp(\pm X_1 i\pi)\Phi_{KZ}(-X_1, -X_0)\text{Li}(z, X_0, X_1) \\ \text{Li}^{\bar{\rho}\bar{\sigma}}(z, X_0, X_1) &= \Phi_{KZ}(X_1 - X_0, -X_0) \exp(\mp X_0 i\pi)\text{Li}(z, X_0, X_1) \end{aligned}$$

and

$$\begin{aligned} &\text{Li}^{\bar{\rho}\bar{\sigma}\bar{\sigma}\bar{\rho}}(z, X_0, X_1) \\ &= \exp(\pm(X_0 - X_1)i\pi)\Phi_{KZ}(X_1 - X_0, -X_0) \exp(\mp X_0 i\pi)\text{Li}(z, X_0, X_1) \\ &= \text{Li}^{\bar{\sigma}\bar{\rho}\bar{\sigma}\bar{\rho}}(z, X_0, X_1) \\ &= \Phi_{KZ}(X_1 - X_0, X_1) \exp(\pm X_1 i\pi)\Phi_{KZ}(-X_1, -X_0)\text{Li}(z, X_0, X_1) \end{aligned}$$

where the ambiguity in sign is according to z being in the upper or lower half plane respectively.

The ambiguity in sign will be resolved in lifting the action to $PSL(2, \mathbb{Z})$.

We remark that the equality $\text{Li}^{\bar{\rho} \circ \bar{\sigma} \circ \bar{\rho}} = \text{Li}^{\bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma}}$ follows from the well-definedness of the Λ action and is a means of using the braid relation $\bar{\rho} \circ \bar{\sigma} \circ \bar{\rho} = \bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma}$ to establish the (highly non-trivial) hexagonal relations of DRINFEL'D, to wit

$$\begin{aligned} & \Phi_{KZ}(X_1 - X_0, X_1) \exp(\pm X_1 i\pi) \Phi_{KZ}(-X_1, -X_0) \\ &= \exp(\pm (X_0 - X_1) i\pi) \Phi_{KZ}(X_1 - X_0, -X_0) \exp(\mp X_0 i\pi). \end{aligned}$$

4. As a first approximation to defining an action of $PSL(2, \mathbb{Z})$ on global sections of \mathcal{P} , pull back to the upper half plane via $\lambda(\tau)$: Given a global section $L(z, X_0, X_1)$ of \mathcal{P} , for every $\tau \in \mathcal{H}$ write $(\lambda^* L)(\tau, X_0, X_1)$ for $L(\lambda(\tau), X_0, X_1)$ then make the

Definition 2.6. If $L(z, X_0, X_1)$ is a global section of \mathcal{U} , $\tau \in \mathcal{H}$, and v is any element of $PSL(2, \mathbb{Z})$ reducing to $\mathcal{A}v$ in $SL(2, \mathbb{Z}/2\mathbb{Z})$, set

$$(\lambda^* L)^v(\tau, X_0, X_1) := (\lambda^* L)(v(\tau), \mathcal{A}v^{-1}X_0, \mathcal{A}v^{-1}X_1)$$

and refer to this as the $PSL(2, \mathbb{Z})$ -action on lifted global sections of \mathcal{U} .

Example 2.7. Let $\sigma \in PSL(2, \mathbb{Z})$ denote the transformation of \mathcal{H} sending τ to $-1/\tau$. As is shown in [Cha80],

$$\lambda(\sigma(\tau)) := \lambda\left(-\frac{1}{\tau}\right) = 1 - \lambda(\tau).$$

Hence

$$\begin{aligned} (\lambda^* \text{Li})^\sigma(\tau, X_0, X_1) &= \text{Li}\left(\lambda\left(-\frac{1}{\tau}\right), -X_1, -X_0\right) \\ &= \text{Li}(\bar{\sigma}\lambda(\tau), \bar{\sigma}^{-1}X_0, \bar{\sigma}^{-1}X_1) \\ &= \Phi_{KZ}(-X_1, -X_0)(\lambda^* \text{Li})(\tau, X_0, X_1) \text{ by E.g. 2.4.} \end{aligned}$$

We would like to interpret the action of σ on $\lambda^* Li$ as some kind of modularity statement for the polylogarithm generating series where the DRINFEL'D associator plays the role of automorphy factor. But more work must be done to achieve this since the action of 2.6 factors through the $SL(2, \mathbb{Z}/2\mathbb{Z})$ action: Indeed, as is obvious from the geometric setup, by using the projection $\mathcal{A} : PSL(2, \mathbb{Z}) \rightarrow SL(2, \mathbb{Z}/2\mathbb{Z})$ one finds

Proposition 2.8. *For any $v \in PSL(2, \mathbb{Z})$,*

$$(\lambda^* L)^v(\tau, X_0, X_1) = L^{\mathcal{A}(v)}(\lambda(\tau), X_0, X_1).$$

Proof. Recall the classical fact

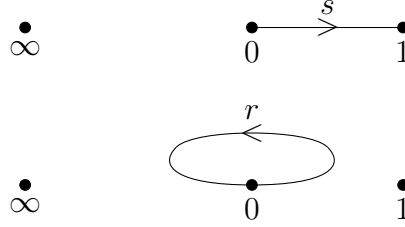
$$\lambda(v(\tau)) = \mathcal{A}(v)(\lambda(\tau))$$

for every $v \in PSL(2, \mathbb{Z})$, proven in [Cha80]. The assertion now follows from the definitions 2.3 and 2.6. \square

3. THE PATH SPACE REALIZATION OF $PSL(2, \mathbb{Z})$

Given a real tangential basepoint \overrightarrow{ab} , the group structure on $PSL(2, \mathbb{Z})$ may be realized on the set $G_{\overrightarrow{ab}}$ (in the notation of 1.1). This idea supplies topological tools with which modularity questions can be investigated.

Consider the case of $\overrightarrow{ab} = \overrightarrow{01}$. Then let s denote the homotopy class of paths in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ represented by the tangential path $[0, 1]$ and let r be the homotopy class of paths represented by the loop from $\overrightarrow{01}$ to $\overrightarrow{0\infty}$ in the upper half plane, as pictured below.



The use of tangential basepoints prevents homotopies which would otherwise occur - in particular, the homotopy classes can detect an *upper half plane* owing to the rigidity of the real line with respect to a choice of a pair of real tangential basepoints. In this way, one sees that r is well-defined as a homotopy class of paths which differs from the class of a similar loop in the lower half plane.

The group structure on $G_{\overrightarrow{ab}}$ is facilitated by the distinct presentations of $SL(2, \mathbb{Z}/2\mathbb{Z})$ coming from (13): Firstly we define the surjection $[\cdot]_{ab}$ of $G_{\overrightarrow{ab}}$ onto $SL(2, \mathbb{Z}/2\mathbb{Z}) \simeq S_3$ by sending a given homotopy class t in $G_{\overrightarrow{ab}}$ with endpoint $\overrightarrow{a_t b_t}$, to the permutation $[t]_{ab}$ of $\{0, 1, \infty\}$ sending a to a_t and b to b_t . Next, we exploit the fact that the fractional linear automorphisms Λ are also isomorphic to $SL(2, \mathbb{Z}/2\mathbb{Z})$ to define an action of this group on $G_{\overrightarrow{ab}}$: Any $\overline{\alpha} \in \Lambda$ is a self-mapping of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ and as such sends any homotopy class u of paths between real tangential basepoints, to some other such homotopy class of paths. We denote the latter by $\overline{\alpha} * u$.

Synthesizing these definitions, we have a map of $G_{\overrightarrow{ab}} \times G_{\overrightarrow{ab}}$ into $G_{\overrightarrow{ab}}$ given by

$$(t, u) \mapsto [t]_{ab} * u.$$

Choosing instead to work with the inverse of the permutation $[t]_{ab}$ gives an equivalent picture, which will later be seen to appear more natural, but only because we are not composing paths in the functional order.

Remark 3.1. When $\overrightarrow{ab} = \overrightarrow{01}$ we write $[\cdot]$ for $[\cdot]_{01}$. Then notice that, viewed as linear fractional transformations of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$,

$$[r] : z \mapsto \frac{z}{z-1}$$

while

$$[s] : z \mapsto 1 - z.$$

Furthermore, for any $t \in G_{\overrightarrow{01}}$ with endpoint $\overrightarrow{a_1 b_1}$, one checks by direct computation that $[t] * r$ may be represented by a loop in the upper or lower half plane (according to the corresponding permutation $[t]$ being even or odd respectively), beginning at $\overrightarrow{a_1 b_1}$ and ending at $\overrightarrow{a_1 c_1}$ where $c_1 \neq b_1$, while $[t] * s$ may be represented by a straight line segment beginning at $\overrightarrow{a_1 b_1}$ and ending at $\overrightarrow{c_1 b_1}$.

Using this action, we define a concatenation procedure for homotopy classes of paths in $G_{\overrightarrow{01}}$ according to the following inductive prescription: If η is a homotopy class of paths formed from the concatenation procedure applied successively to classes in $\{r, s\}$, and ν is either r or s , let $\eta\nu$ be the homotopy class of η followed by $[\eta] * \nu$. Since $[\eta]$ sends ν to a homotopy class of paths originating at the endpoint of the paths in η , it follows that $\eta\nu \in G_{\overrightarrow{01}}$.

The construction may be repeated for any choice of real tangential basepoint \overrightarrow{ab} . In cases other than $\overrightarrow{ab} = \overrightarrow{01}$ write r_{ab} and s_{ab} for the corresponding generators. To be precise, r_{ab} is a loop based at \overrightarrow{ab} of the form of r as above, which is in the upper half plane for $\overrightarrow{ab} = \overrightarrow{\infty 0}$ and $\overrightarrow{ab} = \overrightarrow{1\infty}$ but in the lower half plane when \overrightarrow{ab} is $\overrightarrow{10}$, $\overrightarrow{0\infty}$, or $\overrightarrow{\infty 1}$; while s_{ab} is a straight line segment from \overrightarrow{ab} to \overrightarrow{ba} .

Throughout write \cdot for concatenation of (homotopy classes of) paths.

Definition 3.2. The mapping

$$S_{ab} : G_{\overrightarrow{ab}} \times G_{\overrightarrow{ab}} \rightarrow G_{\overrightarrow{ab}}$$

with

$$S_{ab}(\eta, \mu) = \eta\mu := \eta \cdot ([\eta]_{ab} * \mu)$$

for any $\eta, \mu \in G_{\overrightarrow{ab}}$, will be referred to as $SL(2, \mathbb{Z}/2\mathbb{Z})$ concatenation of tangential paths in $G_{\overrightarrow{ab}}$.

Associativity of successive application of S_{ab} boils down to the

Lemma 3.3. *For any $\eta, \mu \in G_{ab}^{\rightarrow}$,*

$$[\eta\mu] = [\eta] \circ [\mu]$$

Proof. To determine $[\eta\mu] = [\eta \cdot [\eta] * \mu]$ it suffices to find the endpoint of $\eta \cdot [\eta] * \mu$.

Denote the endpoint of η by $\overrightarrow{\eta(a)\eta(b)}$, so that $\eta(a)$ and $\eta(b)$ are the values of a and b respectively under the permutation associated to η by means of which $[\eta]$ is defined. Define $\mu(a)$ and $\mu(b)$ similarly. Then the path $[\eta] * \mu$ sends the basepoint $\overrightarrow{\eta(a)\eta(b)}$ to the image under the transformation $[\eta]$ of $\overrightarrow{\mu(a)\mu(b)}$ - i.e. the endpoint of $\eta \cdot [\eta] * \nu$ is $\overrightarrow{\eta(\mu(a))\eta(\mu(b))}$.

This determines a permutation of $\{0, 1, \infty\}$ giving rise to a transformation of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ which is nothing other than $[\mu]$ followed by $[\eta]$, that is to say $[\eta] \circ [\mu]$. \square

Indeed, we can now prove

Lemma 3.4. *For any η, μ and ν in G_{ab}^{\rightarrow} ,*

$$S_{ab}(\eta, S_{ab}(\mu, \nu)) = S_{ab}(S_{ab}(\eta, \mu), \nu).$$

Proof.

$$\begin{aligned} S_{ab}(\eta, S_{ab}(\mu, \nu)) &= \eta \cdot ([\eta] * (\mu \cdot ([\mu] * \nu))) \\ &= \eta \cdot ([\eta] * \mu) \cdot ([\eta] * ([\mu] * \nu)) \\ &= \eta \cdot ([\eta] * \mu) \cdot (([\eta] \circ [\mu]) * \nu) \\ &= \eta \cdot ([\eta] * \mu) \cdot ([\eta\mu] * \nu) \quad \text{by Lemma 3.3} \\ &= S_{ab}(S_{ab}(\eta, \mu), \nu) \end{aligned}$$

\square

Because of the associativity, for any $n \geq 1$, the $SL(2, \mathbb{Z}/2\mathbb{Z})$ concatenation $\nu_1 \dots \nu_n$ of elements $\nu_j \in \{r, s\}$ is uniquely determined. It is given by

$$\nu_1 \cdot ([\nu_1] * \nu_2) \cdot ([\nu_1 \cdot [\nu_1] * \nu_2] * \nu_3) \cdot \dots \cdot ([\nu_1 \cdot [\nu_1] * \nu_2 \cdot \dots \cdot ([\nu_1 \cdot [\nu_1] * \nu_2] * \nu_3) \cdot \dots] * \nu_{n-1}) * \nu_n,$$

where \cdot again denotes concatenation of (homotopy classes of) paths.

Applying Lemma 3.3 iteratively, one sees that for any $m \leq n$,

$$[\nu_1 \dots \nu_m] = [\nu_1] \circ \dots \circ [\nu_m],$$

so $\nu_1 \dots \nu_n$ may be rewritten

$$\nu_1 \cdot ([\nu_1] * \nu_2) \cdot (([\nu_1] \circ [\nu_2]) * \nu_3) \cdot \dots \cdot (([\nu_1] \circ \dots \circ [\nu_{n-1}]) * \nu_n).$$

Theorem 3.5. *For any real tangential basepoint \overrightarrow{ab} , $G_{\overrightarrow{ab}}$ may be endowed with a group structure with multiplication given by S_{ab} .*

Proof. It suffices to consider the case of $\overrightarrow{ab} = \overrightarrow{01}$.

Associativity of the multiplication was established in Lemma 3.4.

Begin by observing that the class e of the trivial path acts as the identity. Also, s is its own inverse, since $[s] * s$ is the homotopy class of paths represented by the tangential path $[1, 0]$, which is inverse to $[0, 1]$. The inverse of r is the homotopy class q of paths represented by the loop from $\overrightarrow{01}$ to $\overrightarrow{0\infty}$ in the lower half plane - one checks easily that $rq = qr = e$. We write $q = r^{-1}$. A key fact is that $[r] = [r^{-1}]$, as one sees directly from the definition of $[\cdot]$.

Now for arbitrary $\nu_j \in \{r, s\}$, the product $\nu_1 \dots \nu_n$ has as inverse $\nu_n^{-1} \dots \nu_1^{-1}$: Suppose that it is known that $\nu_1 \dots \nu_k \nu_k^{-1} \dots \nu_1^{-1} = e$, for all possible ν_j and $k \leq N - 1$. Then for arbitrary $\nu_j \in \{r, s\}$ consider

$$\begin{aligned} & \nu_1 \dots \nu_N \nu_N^{-1} \dots \nu_1^{-1} \\ = & \nu_1 \cdot \dots ([\nu_1] * \nu_2) \cdot (([\nu_1] \circ [\nu_2]) * \nu_3) \cdot \dots \\ & (([\nu_1] \circ \dots \circ [\nu_{N-1}]) * \nu_N) \cdot (([\nu_1] \circ \dots \circ [\nu_N]) * \nu_N^{-1}) \cdot \\ & (([\nu_1] \circ \dots \circ [\nu_N] \circ [\nu_N^{-1}]) * \nu_{N-1}^{-1}) \cdot \dots (([\nu_1] \circ \dots \circ [\nu_3^{-1}] \circ [\nu_2^{-1}]) * \nu_1^{-1}). \end{aligned}$$

From the definition of $[\cdot]$, one finds that

$$(16) \quad ([\nu_1] \circ \dots \circ [\nu_{N-1}]) * \nu_N \cdot (([\nu_1] \circ \dots \circ [\nu_{N-1}]) \circ [\nu_N] * \nu_N^{-1}) = e.$$

The fact that $[r]$ and $[s]$ are involutions implies that for any j , $[\nu_j] \circ [\nu_j^{-1}] = 1$, the identity morphism on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. When combined with (16), this shows that

$$\nu_1 \dots \nu_N \nu_N^{-1} \dots \nu_1^{-1} = \nu_1 \dots \nu_{N-1} \nu_{N-1}^{-1} \dots \nu_1^{-1}$$

which is trivial by the inductive hypothesis. \square

Theorem 3.6. *With the group structure of Theorem 3.5,*

$$G_{\overrightarrow{ab}} \simeq \langle r_{ab}, s_{ab} \rangle / (s_{ab}^2, (s_{ab} r_{ab})^3),$$

where $\langle r_{ab}, s_{ab} \rangle = F_2$ denotes the free group on the two generators r_{ab} and s_{ab} .

Proof. Any given homotopy class of paths in $G_{\overrightarrow{ab}}$ may be decomposed as a succession of loops of the form of r_{ab} and straight lines of the form of s_{ab} , so it is clear from Remark 3.1 that the elements of $\{r_{ab}, s_{ab}\}$ generate the group $G_{\overrightarrow{ab}}$.

It again suffices to consider only the case $\overrightarrow{ab} = \overrightarrow{01}$.

Write $G_{\vec{01}} \simeq \langle r, s \rangle / I_{01}$ for some family of relations I_{01} .

From the definitions one sees that as homotopy classes of paths in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, s^2 is the trivial class, as are $sr sr sr$, $sr^{-1} sr^{-1} sr^{-1}$, $rs rs rs$ and $r^{-1} sr^{-1} sr^{-1} s$. Observe that the last four relations may be summarised by $(sr)^3 = 1$ since $s^2 = 1$. Thus we know that $(s^2, (sr)^3) \subseteq I_{01}$ so it remains to establish the reverse inclusion.

$G_{\vec{01}}$ surjects onto $SL(2, \mathbb{Z}/2\mathbb{Z})$, which as in (13) is isomorphic to

$$\langle \bar{\rho}, \bar{\sigma} | \bar{\rho}^2 = \bar{\sigma}^2 = 1, \bar{\rho}\bar{\sigma}\bar{\rho} = \bar{\sigma}\bar{\rho}\bar{\sigma} \rangle,$$

by sending r to $\bar{\rho}$ and s to $\bar{\sigma}$. Since the kernel is exactly $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \vec{01})$, which embeds into $G_{\vec{01}}$ as $\langle r^2, sr^2s \rangle$, we have the short exact sequence

$$1 \rightarrow \langle r^2, sr^2s \rangle \rightarrow \langle r, s \rangle / I_{01} \rightarrow \langle \bar{\rho}, \bar{\sigma} \rangle / (\bar{\rho}^2, \bar{\sigma}^2, \bar{\sigma}\bar{\rho}\bar{\sigma}\bar{\rho}\bar{\sigma}) \rightarrow 1.$$

Then I_{01} is contained in the lift J_{01} of $(\bar{\rho}^2, \bar{\sigma}^2, \bar{\sigma}\bar{\rho}\bar{\sigma}\bar{\rho}\bar{\sigma})$ to $G_{\vec{01}}$, which coincides with $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \vec{01})$ as embedded into $G_{\vec{01}}$.

Now the lift of an element $\bar{\mu}_1 \dots \bar{\mu}_n$ of $SL(2, \mathbb{Z}/2\mathbb{Z})$ (with $\bar{\mu}_j \in \{\bar{\rho}, \bar{\sigma}\}$ for each j) to $G_{\vec{01}}$ is of the form of $u_1 m_1 \dots u_n m_n u_{n+1}$ where the $u_j \in \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \vec{a_j b_j})$ for suitable $a_j, b_j \in \{0, 1, \infty\}$, for $j = 1, \dots, n+1$ and

$$m_j = \begin{cases} r & \text{if } \bar{\mu}_j = \bar{\rho}; \\ s & \text{if } \bar{\mu}_j = \bar{\sigma}. \end{cases}$$

Since the fundamental group is free, it thus suffices to show that each element of J_{01} given in the above notation by $m_1 u_2 \dots u_n m_n$, may be expressed in terms of the generators r^2 and sr^2s using only the known relations mentioned above, in order to conclude that no other relations exist in I_{01} .

Begin by considering the subgroup B_{01} of J_{01} generated by the eight elements $sr^{\delta_1} sr^{\delta_2} sr^{\delta_3}$ where for $j = 1, 2, 3$, δ_j is either 1 or -1 . Of these generators, we have seen that $sr sr sr$ and $sr^{-1} sr^{-1} sr^{-1}$ are trivial. For the rest, recall the relations $sr sr sr = 1$ and $sr^{-1} sr^{-1} sr^{-1} = 1$, from which we know that $srs \sim r^{-1} sr^{-1}$ and $sr^{-1} s \sim r sr$, and compute:

$$\begin{aligned} sr sr^{-1} sr^{-1} &= srs(srs) = sr^2s \\ sr sr^{-1} sr &= sr(rsr)r = sr^2sr^2 \\ sr sr sr^{-1} &= (r^{-1} sr^{-1})r sr^{-1} = r^{-2} \\ sr^{-1} sr sr &= sr^{-1}s(sr^{-1}s) = sr^{-2}s \\ sr^{-1} sr^{-1} sr &= s(srs)sr = r^2 \\ sr^{-1} sr sr^{-1} &= sr^{-1}(r^{-1} sr^{-1})r^{-1} = sr^{-2}sr^{-2}. \end{aligned}$$

Since the known relations are the only ones needed to rewrite the generators of B_{01} in terms of those of J_{01} , necessarily the only relations among generators of B_{01} follow from $s^2 = 1$ and $(sr)^3 = 1$. This can also be verified directly: For example, that the inverse of $sr sr sr^{-1} = r^{-2}$ is $sr^{-1} sr^{-1} sr = r^2$ follows from the known relation $sr^{-1} sr^{-1} sr^{-1} = 1$, (which implies both $sr^{-1} sr^{-1} = rs$ and $r^{-1} sr^{-1} s = sr$) since

$$sr^{-1} sr^{-1} sr = (sr^{-1} sr^{-1})(sr) = (rs)(r^{-1} sr^{-1} s) = (sr sr sr^{-1})^{-1}.$$

Similar calculations may be performed with respect to any other pair of generators of B_{01} , and are left to the reader.

Notice that since $sr^{-1} sr^{-1} sr = r^2$ and $sr sr^{-1} sr^{-1} = sr^2 s$, B_{01} is in fact isomorphic to $J_{01} \simeq \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{01})$.

Now consider a lift $rt_1 r$ of $\vec{\rho}^2$ to G_{01} , where t_1 is a closed loop based at $\overrightarrow{0\infty}$. If $t_1 = r^{2n} t_2$ (case 1) where t_2 is another such loop based at $\overrightarrow{0\infty}$, then

$$rt_1 r = r^{2n}(rt_2 r)$$

where t_2 is a word in the symbols $x_0 := r^2$ and $x_1 := sr^2 s$ of length strictly less than that of t_1 .

If $t_1 = sr^2 s \cdot t_2$ (case 2) where t_2 is another element of $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{0\infty})$, then

$$rt_1 r = (rsr)rst_2 r = sr^{-1} sr st_2 r.$$

If $t_2 = 1$, (subcase 2.i) then $rt_1 r = sr^{-1} sr sr = sr^{-2} s$ as computed above. Otherwise, the loop t_2 is either of the form of $r^2 t_3$ (subcase 2.ii) or $sr^2 st_3$ (subcase 2.iii) for suitable t_3 . In subcase 2.ii,

$$rt_1 r = (sr^{-1} sr sr)rt_3 r = (sr^{-2} s)rt_3 r$$

where we use the expression for $sr^{-1} sr sr$ computed above. Here, t_3 is a word in x_0 and x_1 again of length strictly less than that of t_1 , so repeating the argument for $rt_3 r$ leads to a similar shorter word t_4 or to the subcase 2.iii.

In subcase 2.iii:

$$\begin{aligned} rt_1 r &= sr^{-1} sr sr^2 st_3 r &&= sr^{-1} (sr s) sr^2 st_3 r \\ &= sr^{-1} (r^{-1} sr^{-1}) sr^2 st_3 r &&= (sr^{-2} s) (r^{-1} s) r ssr st_3 r \\ &= (sr^{-2} s) sr sr s (sr s) sr st_3 r &&= (sr^{-2} s) sr sr s (r^{-1} sr^{-1}) sr st_3 r \\ &= (sr^{-2} s) (r^{-2}) sr^{-1} sr st_3 r \end{aligned}$$

where the expression for the generator $sr sr sr^{-1} = r^{-2}$ of B_{01} has been used, along with the known relations. In the final expression, s precedes t_3 as s precedes t_2 in $t_1 = sr^2 st_2$. Again here, t_3 is a word in the x_0 and x_1 which is shorter than t_2 , which in turn is shorter than t_1 .

Since t_1 is a finite word, regardless of which cases occur, this procedure terminates after finitely many steps with some word $t_k = 1$, which is handled as before in subcase 2.i. In this way, rt_1r is expressed explicitly as some word t'_1 in the generators r^2 and sr^2s of the fundamental group. In particular, we have

$$(17) \quad rt_1 = t'_1 r^{-1}.$$

Now it is clear by an inductive argument that elements of J_{01} of the form of $ru_1ru_2 \dots u_{2n-1}r$ and $r^{-1}u_1r^{-1}u_2 \dots u_{2n-1}r^{-1}$ (with notation as above - i.e. the u_j are elements of suitable fundamental groups) may similarly be expressed in terms of elements $sr^{\pm 2}s$ and $r^{\pm 2}$ of the fundamental group using only the relations $s^2 = 1$ and $(sr)^3 = 1$.

Next consider sus for any $u \in \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{10})$. By a simpler analysis to the above, (indeed, using only $s^2 = 1$), it is possible to determine the explicit $u' \in \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{01})$ in terms of the generators r^2 and sr^2s for which $sus = u'$, or stated otherwise,

$$(18) \quad su = u's.$$

It remains to verify the same for the words of the form of

$$su_1r^{\delta_1}t_1su_2r^{\delta_2}t_2su_3r^{\delta_3}t_3$$

where δ_j is either 1 or -1 for $j = 1, 2, 3$ and the u_j and t_j are elements of suitable fundamental groups. But it is clear that using (17) and (18) repeatedly one can write

$$su_1r^{\delta_1}t_1su_2r^{\delta_2}t_2su_3r^{\delta_3}t_3 = v sr^{-\delta_1} sr^{-\delta_2} sr^{-\delta_3}$$

where v is some (explicit) word in the $r^{\pm 2}$ and $sr^{\pm 2}s$, as is $sr^{-\delta_1} sr^{-\delta_2} sr^{-\delta_3}$. \square

Lemma 3.7. *If \overrightarrow{ab} is a real tangential baspoint for which $G_{\overrightarrow{ab}}$ is endowed with the group structure of the Theorem 3.5, then*

$$\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{ab}) \triangleleft G_{\overrightarrow{ab}}.$$

The proof is trivial, especially in light of the

Proposition 3.8.

$$PSL(2, \mathbb{Z}) = \langle \rho, \sigma \rangle / (\sigma^2, (\rho \circ \sigma)^3)$$

where $\langle \rho, \sigma \rangle = F_2$, the free group on two generators.

Proof. Using the BRUHAT decomposition, one can write down generators and relations for $SL(2, \mathbb{R})$. See [Lan85], for example. In $PSL(2, \mathbb{Z})$

(regarded as the group of linear fractional transformations of \mathcal{H}), these amount to generators

$$\rho : \tau \mapsto 1 + \tau$$

and

$$\sigma : \tau \mapsto -\frac{1}{\tau}$$

with the relations $\sigma^2 = I$ and $(\sigma \circ \rho^{-1})^3 = I$. \square

Corollary 3.9. *For any real tangential basepoint \overrightarrow{ab} ,*

$$PSL(2, \mathbb{Z}) \simeq G_{\overrightarrow{ab}}$$

Proof. Combine Proposition 3.8 with Theorem 3.5. \square

As a further instance of the welding of topological and algebraic perspectives so ubiquitous in this subject, this isomorphism expresses a fundamental duality between homotopy classes of paths in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ and projective classes of matrices of $SL(2, \mathbb{Z})$. It is likely that deformations of matrices of $SL(2, \mathbb{R})$ can be made to correspond with deformations of paths within the same homotopy class - i.e. it should be possible to endow $SL(2, \mathbb{R})$ with a notion of homotopy equivalence corresponding to deformation of matrices.

Notational remark 3.10. The multiplication in $PSL(2, \mathbb{Z})$ is written in the functional order, whereas concatenation of paths in $G_{\overrightarrow{ab}}$ occurs in the order in which the paths are written.

Remark 3.11. Denote the isomorphism of Corollary 3.9 by

$$\Psi_{ab} : G_{\overrightarrow{ab}} \xrightarrow{\cong} PSL(2, \mathbb{Z}),$$

writing $\Psi := \Psi_{01}$ in the special case of $\overrightarrow{ab} = \overrightarrow{01}$. Concretely, we have the following correspondences:

$$\Psi_{ab}(r_{ab}) = (\rho : \tau \mapsto \tau + 1)$$

$$\Psi_{ab}(s_{ab}) = (\sigma : \tau \mapsto -\frac{1}{\tau})$$

$$\Psi_{ab}(r_{ab}^2) = (\rho^2 : \tau \mapsto \tau + 2)$$

$$\Psi_{ab}(s_{ab} r_{ab}^2 s_{ab}) = (\sigma \circ \rho^2 \circ \sigma : \tau \mapsto \frac{\tau}{1 - 2\tau})$$

Recall that $\Gamma(2)/\{\pm I\} = \langle \rho^2, \sigma \circ \rho^2 \circ \sigma \rangle$, and notice here that r^2 is represented by a loop about 0 based at $\overrightarrow{01}$ while sr^2s is represented by a loop about 1 based at $\overrightarrow{01}$, which together generate $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{01})$. In this way, we have expressed the isomorphism of the fundamental group with the congruence subgroup on the level of the generators. But the fundamental domain for $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ in \mathcal{H} (see [Cha80]) exhibits some symmetries with respect to the generators of $PSL(2, \mathbb{Z})$ itself: σ expresses the symmetry of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ around the line $\Re(z) = \frac{1}{2}$, which under the $\lambda(\tau)$ of §2 lifts to the portion of the unit circle in \mathcal{H} and its translates under $\Gamma(2)/\{\pm I\}$. At the same time, ρ expresses the symmetry about the circle $\{1 + e^{i\theta} | 0 \leq \theta < 2\pi\}$, which again lifts under $\lambda(\tau)$ to a family of curves enclosing regions which together with their translates under ρ , tile \mathcal{H} . In both cases, a fundamental domain \mathfrak{F} for the covering may be chosen so that the region C enclosed by a specific lift of the path of symmetry in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ has $\mathfrak{F} = C \cup \alpha(C)$ for $\alpha = \sigma, \rho$, where the union is disjoint but for points of the lift of the path itself. On another level, observe that the lift of s under λ gives a family of paths of \mathcal{H} which are exactly the geodesics mapped into themselves by the involution σ , namely the imaginary axis and its translates under $\Gamma(2)$.

Theorem 3.12. *For any given $u \in G_{\overrightarrow{ab}}$, $\Psi_{ab}(u)$ is a transformation of the upper half plane which sends the lift of \overrightarrow{ab} under $\lambda(\tau)$ in some fixed fundamental domain for $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, to some lift of the endpoint of u under $\lambda(\tau)$.*

Proof. Knowing the action of λ on the boundary of a fundamental domain for $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ in \mathcal{H} (see [Cha80]) is enough to check this directly for the generators r_{ab} and s_{ab} of $G_{\overrightarrow{ab}}$, as one may do with no difficulty. Having established the assertion for r_{ab} and s_{ab} for *all* real tangential basepoints \overrightarrow{ab} suffices to prove the theorem for general u , because multiplication in $G_{\overrightarrow{ab}}$ is performed by means of concatenation of paths, each of which necessarily begins at the endpoint of the previous path, and the corresponding successive transformations in the upper half plane are all maps sending the lift of some \overrightarrow{cd} to the lift of the endpoint of either r_{cd} or s_{cd} for some $c, d \in \{0, 1, \infty\}$. \square

Corollary 3.13. *For any real tangential basepoint \overrightarrow{ab} ,*

$$[\Psi_{ab}^{-1}(\cdot)]_{ab} : PSL(2, \mathbb{Z}) \rightarrow SL(2, \mathbb{Z}/2\mathbb{Z})$$

is the usual projection (i.e. \mathcal{A} of (12)).

Proof. This follows immediately from Theorem 3.12: Indeed, the mapping associating to the transformation $v \in PSL(2, \mathbb{Z})$ the endpoint of $\Psi_{ab}^{-1}(v) \in G_{\vec{ab}}$ (which determines $[\Psi_{ab}^{-1}(v)]_{ab}$), is determined by $\lambda(\tau)$, so goes according to $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \vec{ab})$ conjugacy classes. Now refer to (12) to see that these conjugacy classes correspond exactly to the elements of $SL(2, \mathbb{Z}/2\mathbb{Z})$. \square

The corollary is also evident from the short exact sequence appearing in the proof of Theorem 3.6.

Notice that $[\cdot]$ does not play an explicit role in the description of multiplication in $PSL(2, \mathbb{Z})$, which is the usual composition of MÖBIUS transformations.

Subsequently write $\mathcal{A}(v) = \bar{v}$ for any $v \in PSL(2, \mathbb{Z})$.

4. QUASI-MODULARITY AND THE LIFTED ACTION ON SECTIONS OF \mathcal{U}

4.1. The $PSL(2, \mathbb{Z})$ action.

4.1.1. *Actions on power series.* Recall the action of $SL(2, \mathbb{Z}/2\mathbb{Z})$ on the formal variables X_0 and X_1 as given in the table in §2. This extends by linearity to polynomials in the X_j with complex coefficients, and thereby to the quotients

$$\mathbb{C} \langle X_0, X_1 \rangle / I^{N+1}$$

(where $I = (X_0, X_1)$ denotes the augmentation ideal), and hence to the inverse limit $\mathbb{C} \ll X_0, X_1 \gg$.

Likewise based on the action on the formal variables X_0 and X_1 of §2, a different action of $SL(2, \mathbb{Z}/2\mathbb{Z})$ on formal power series in these variables emerges naturally in investigating the action on sections of \mathcal{U} of §2 lifted to $PSL(2, \mathbb{Z})$.

Definition 4.1. The action of $\bar{\alpha} \in SL(2, \mathbb{Z}/2\mathbb{Z})$ on a formal power series $F(X_0, X_1) \in \mathbb{C} \ll X_0, X_1 \gg$ is given by

$$F(X_0, X_1)^{\bar{\alpha}} := F(\bar{\alpha}^{-1}X_0, \bar{\alpha}^{-1}X_1).$$

Notice that then, for any $\bar{\beta} \in SL(2, \mathbb{Z}/2\mathbb{Z})$,

$$F(X_0, X_1)^{\bar{\alpha}\bar{\beta}} = F(\bar{\beta}^{-1}X_0, \bar{\beta}^{-1}X_1)^{\bar{\alpha}} = F(\bar{\beta}^{-1} \circ \bar{\alpha}^{-1}X_0, \bar{\beta}^{-1} \circ \bar{\alpha}^{-1}X_1).$$

A given element $\alpha \in PSL(2, \mathbb{Z})$ then acts on power series by reduction to $SL(2, \mathbb{Z}/2\mathbb{Z})$. In this case we replace $\bar{\alpha}$ by α in the notation for the

above action -i.e. we set

$$(19) \quad F(X_0, X_1)^\alpha := F(X_0, X_1)^{\bar{\alpha}}.$$

4.1.2. *Action on sections of \mathcal{U} .* Let V_c be some open neighbourhood of $c \in \{0, 1, \infty\}$ in \mathbb{P}^1 for which $(V_c \setminus \{c\}) \cap \{0, 1, \infty\}$ is empty. Then set $U_c := V_c \setminus \{c\}$. This is an open set of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$.

Suppose that $L_a(z, X_0, X_1)$ is a section of (\mathcal{U}, ∇) defined over U_a - i.e. $L_a(z, X_0, X_1) \in \Gamma(U_a, \mathcal{U})$. As above, let \bar{v} denote the image of $v \in PSL(2, \mathbb{Z})$ under the usual projection map to $SL(2, \mathbb{Z}/2\mathbb{Z})$. Then by Definition 2.3,

$$L_a^{\bar{v}}(z, X_0, X_1) = L_a(\bar{v}z, X_0, X_1)$$

gives the $SL(2, \mathbb{Z}/2\mathbb{Z})$ action on sections of \mathcal{U} . We lift this to an action of $PSL(2, \mathbb{Z})$ by using the identification of the elements of $PSL(2, \mathbb{Z})$ with those of $G_{\vec{ab}}$ (as in Corollary 3.9), as follows:

Definition 4.2. Given $v \in PSL(2, \mathbb{Z})$, analytically continue $L_a(z, X_0, X_1)$ along the $u \in G_{\vec{ab}}$ corresponding to v , and in the expression which results replace X_j by $\bar{v}^{-1}X_j$ for $j = 0, 1$. This is an action of $PSL(2, \mathbb{Z})$ for which the image of $L_a(z, X_0, X_1)$ will be denoted by

$$L_a^v(z, X_0, X_1).$$

A priori, this action sends $\Gamma(U_a, \mathcal{U})$ into

$$\Gamma_{01\infty} := \cup_{c \in \{0, 1, \infty\}} \Gamma(U_c, \mathcal{U}),$$

but later we will see that the image is contained in $\Gamma(U_a, \mathcal{U})$ itself.

4.2. Quasi-modularity.

Definition 4.3. A local section $L(z, X_0, X_1) \in \Gamma(U_a, \mathcal{U})$ is *quasi-modular* with respect to the congruence subgroup $\Gamma < PSL(2, \mathbb{Z})$ if for every $v \in \Gamma$,

$$(20) \quad L^v(z, X_0, X_1) = K_v(X_0, X_1)L(z, X_0, X_1)$$

for some formal power series $K_v(X_0, X_1)$ such that

$$K_\bullet(X_0, X_1) : \Gamma \rightarrow \mathbb{C} \langle\langle X_0, X_1 \rangle\rangle^\times$$

is a 1-cocycle with respect to the action of $SL(2, \mathbb{Z}/2\mathbb{Z})$ on $\mathbb{C} \langle\langle X_0, X_1 \rangle\rangle^\times$ of Definition 4.1. Such a $K_\bullet(X_0, X_1)$ will be referred to as a *quasi-automorphy factor*.

Now for any $L(z, X_0, X_1)$ satisfying (20) for some family $K_\bullet(X_0, X_1)$ of power series, and for any v, v' in Γ , it is immediate that

$$(L^v)^{v'}(z, X_0, X_1) = K_v(X_0, X_1)^{v'} L^{v'}(z, X_0, X_1),$$

so as usual the cocycle requirement ensures that

$$(L^v)^{v'}(z, X_0, X_1) = L^{v' \circ v}(z, X_0, X_1)$$

for any $v, v' \in \Gamma$, giving a *group action* of Γ on some space of sections.

4.2.1. *Quasi-modularity of $\text{Li}(z)$.* The aim of this subsection is to show that $\text{Li}(z)$ is quasi-modular with respect to $PSL(2, \mathbb{Z})$, and to compute the associated quasi-automorphy factor.

Begin by setting

$$\omega(X_0, X_1) := \frac{dz}{z} X_0 + \frac{dz}{1-z} X_1$$

and write

$$\omega(X_0, X_1)^\alpha = \omega(\bar{\alpha}^{-1} X_0, \bar{\alpha}^{-1} X_1).$$

The following result will prove to be essential:

Lemma 4.4. *For any $\alpha \in PSL(2, \mathbb{Z})$,*

$$\bar{\alpha}^* \omega(X_0, X_1) := \left[\bar{\alpha}^* \left(\frac{dz}{z} \right) \right] X_0 + \left[\bar{\alpha}^* \left(\frac{dz}{1-z} \right) \right] X_1 = \omega(\bar{\alpha} X_0, \bar{\alpha} X_1).$$

Proof. One checks this directly by an elementary computation for each $\bar{\alpha} \in SL(2, \mathbb{Z}/2\mathbb{Z}) \simeq \Lambda$. This verification is equivalent to the simple computation of the $\bar{\alpha}$ action on (X_0, X_1) as given in §2. \square

A related fact which explains the suitability of Definition 4.1 is the

Lemma 4.5. *For any $\alpha, \beta \in PSL(2, \mathbb{Z})$,*

$$\bar{\alpha}^* \omega(\bar{\beta} X_0, \bar{\beta} X_1) := \left[\bar{\alpha}^* \left(\frac{dz}{z} \right) \right] \bar{\beta} X_0 + \left[\bar{\alpha}^* \left(\frac{dz}{1-z} \right) \right] \bar{\beta} X_1 = \omega(\bar{\beta} \circ \bar{\alpha} X_0, \bar{\beta} \circ \bar{\alpha} X_1).$$

Proof. This follows from the previous lemma by using the linearity of $\bar{\beta}$. \square

Now let $\int_\alpha \tilde{\omega}^n$ denote the n -fold CHEN iterated integral of the form $\tilde{\omega}$ along α - i.e. an iterated integral in which $\tilde{\omega}$ is repeated n times. Also write $\int_\alpha \tilde{\omega}^0 = 1$. Then we have

Theorem 4.6. *For any $\alpha \in PSL(2, \mathbb{Z})$,*

$$\mathrm{Li}^\alpha(z, X_0, X_1) = F_\alpha(X_0, X_1) \mathrm{Li}(z, X_0, X_1)$$

where $F_\alpha(X_0, X_1)$ is a formal power series given by the CHEN series

$$F_\alpha(X_0, X_1) := \sum_{n \geq 0} \int_{\Psi^{-1}\alpha} \omega(Y_0, Y_1)^n \Big|_{Y_j = \bar{\alpha}^{-1} X_j : j=0,1}.$$

Implicitly here, $PSL(2, \mathbb{Z})$ is identified with $G_{\vec{0}\vec{1}}$. Also, the notation in the definition of $F_\alpha(X_0, X_1)$ is meant to suggest that the expressions $\bar{\alpha}^{-1} X_j$ for $j = 0, 1$ must be substituted after the integral has been computed. (This changes the power series obtained when one considers for example $F_{\alpha \circ \beta}(X_0, X_1)$ for $\alpha, \beta \in PSL(2, \mathbb{Z})$.)

Proof. When the CHEN iterated integrals are suitably interpreted - regularizing $\frac{dz}{z}$ at $z = 0$ and $\frac{dz}{1-z}$ at $z = 1$ in the usual way (cf. [Joy10]) - for $z \notin (-\infty, 0) \cup (1, \infty)$ the polylogarithm generating function may be expressed as

$$\mathrm{Li}(z, X_0, X_1) = \sum_{n \geq 0} \int_{[\vec{0}\vec{1}, z]} \omega(X_0, X_1)^n$$

where $[\vec{0}\vec{1}, z]$ is a path from the tangential base point $\vec{0}\vec{1}$ to z which does not cut the real axis, (unless $z \in (0, 1)$, in which case the path lies along the real axis).

Now consider $\Psi^{-1}(\alpha) \in G_{\vec{0}\vec{1}}$. Denote the endpoint thereof by \vec{cd} , and a path from \vec{cd} to $\bar{\alpha}z$ which does not cross the real axis by $[\vec{cd}, \bar{\alpha}z]$. Then composing paths in the order as written (i.e. not the functional order), the analytic continuation of $\mathrm{Li}(z, X_0, X_1)$ along $\Psi^{-1}(\alpha)$ is given by

$$\sum_{n \geq 0} \int_{\Psi^{-1}\alpha \cdot [\vec{cd}, \bar{\alpha}(z)]} \omega(X_0, X_1)^n.$$

Consider a typical integral which appears here. Using the coproduct formula for iterated integrals (since $\omega(X_0, X_1)$ is a 1-form),

$$\begin{aligned} & \int_{\Psi^{-1}\alpha \cdot [\vec{cd}, \bar{\alpha}z]} \omega(X_0, X_1)^n \\ &= \sum_{k=0}^n \int_{\Psi^{-1}\alpha} \omega(X_0, X_1)^k \cdot \int_{[\vec{cd}, \bar{\alpha}z]} \omega(X_0, X_1)^{n-k}. \end{aligned}$$

Now

$$\begin{aligned} \int_{[\vec{cd}, \vec{\alpha z}]} \omega(X_0, X_1)^{n-k} &= \int_{[\vec{01}, z]} \bar{\alpha}^* \omega(X_0, X_1)^{n-k} \\ &= \int_{[\vec{01}, z]} \omega(\bar{\alpha} X_0, \bar{\alpha} X_1)^{n-k} \end{aligned}$$

by the Lemma 4.4. Hence $\text{Li}^\alpha(z, X_0, X_1)$ is the same as

$$\begin{aligned} &\left[\sum_{n \geq 0} \sum_{k=0}^n \int_{\Psi^{-1}\alpha} \omega(Y_0, Y_1)^k \cdot \int_{[\vec{01}, z]} \omega(\bar{\alpha} Y_0, \bar{\alpha} Y_1)^{n-k} \right] \Big|_{Y_j = \bar{\alpha}^{-1} X_j; j=0,1} \\ &= \left[\sum_{n \geq 0} \int_{\Psi^{-1}\alpha} \omega(Y_0, Y_1)^n \Big|_{Y_j = \bar{\alpha}^{-1} X_j; j=0,1} \right] \cdot \text{Li}(z, X_0, X_1). \end{aligned}$$

□

Now we can prove the fundamental

Corollary 4.7.

$$\text{Li}^\rho(z, X_0, X_1) = \exp(i\pi X_0) \text{Li}(z, X_0, X_1)$$

$$\text{Li}^\sigma(z, X_0, X_1) = \Phi_{KZ}(X_0, X_1)^\sigma \text{Li}(z, X_0, X_1)$$

Proof. Recall that $\Psi(r) = \rho$ and $\Psi(s) = \sigma$ in the notation of §3. Also, $\bar{\rho}(X_0, X_1) = (X_0, X_0 - X_1)$ while $\bar{\sigma}(X_0, X_1) = (-X_1, -X_0)$.

One computes

$$\int_r \left(\frac{dz}{z} X_0 + \frac{dz}{1-z} X_1 \right)^n = (i\pi X_0)^n$$

since the integrals in which $\frac{dz}{1-z}$ occur vanish along r . Thence

$$\begin{aligned} F_\rho(X_0, X_1) &= \sum_{n=0}^{\infty} \int_r \left(\frac{dz}{z} X_0 + \frac{dz}{1-z} (X_0 - X_1) \right)^n \\ &= \sum_{n=0}^{\infty} (i\pi X_0)^n \\ &= \exp i\pi X_0. \end{aligned}$$

It is well-known that

$$\Phi_{KZ}(X_0, X_1) = \sum_{n=0}^{\infty} \int_{[0,1]} \left(\frac{dz}{z} X_0 + \frac{dz}{1-z} X_1 \right)^n,$$

(see [Car01] for example), in which expression we understand the integrals to be suitably regularized as before. From Theorem 4.6 the second assertion of the corollary follows. \square

The power series which arise here do not look too different from those which result in the case of the $SL(2, \mathbb{Z}/2\mathbb{Z})$ action as in §2. Where σ is concerned, the reason for this is that $\bar{\sigma}$ has a unique lift to $PSL(2, \mathbb{Z})$. On the other hand, unlike that of $\bar{\rho}$ the action of ρ is not involutive.

$F_\bullet(X_0, X_1)$ is a quasi-automorphy factor:

Theorem 4.8. *$F_\bullet(X_0, X_1)$ is a 1-cocycle for $PSL(2, \mathbb{Z})$ in the multiplicative group of formal power series in the non-commuting variables X_0 and X_1 equipped with the action of $SL(2, \mathbb{Z}/2\mathbb{Z})$. Specifically, for any $v, v' \in PSL(2, \mathbb{Z})$,*

$$F_v(X_0, X_1)^{v'} F_{v'}(X_0, X_1) = F_{v' \circ v}(X_0, X_1).$$

Proof. Consider such arbitrary v and $v' \in PSL(2, \mathbb{Z})$ and write $u := \Psi_{ab}^{-1}(v)$ and $u' := \Psi_{ab}^{-1}(v')$. Also, interpret $\int_v \omega^0$ as 1 so that

$$F_{v' \circ v}(X_0, X_1) = \sum_{n=0}^{\infty} \int_{uu'} \left(\frac{dz}{z} Y_0 + \frac{dz}{1-z} Y_1 \right)^n \Big|_{Y_j = \bar{v}^{-1} \circ \bar{v}'^{-1} X_j : j=0,1}$$

Now recall from §3 that $uu' = u \cdot [u] * u'$, and use the coproduct formula for iterated integrals to compute

$$\begin{aligned} \int_{uu'} \left(\frac{dz}{z} Y_0 + \frac{dz}{1-z} Y_1 \right)^n &= \sum_{k=0}^n \int_u \omega(Y_0, Y_1)^k \int_{[u]*u'} \omega(Y_0, Y_1)^{n-k} \\ &= \sum_{k=0}^n \int_u \omega(Y_0, Y_1)^k \int_{u'} \bar{v}^* \omega(Y_0, Y_1)^{n-k} \\ &= \sum_{k=0}^n \int_u \omega(Y_0, Y_1)^k \int_{u'} \omega(\bar{v} Y_0, \bar{v} Y_1)^{n-k} \end{aligned}$$

using Lemma 4.4 and Corollary 3.13. Hence

$$\begin{aligned} F_{v' \circ v}(X_0, X_1) &= \sum_{n \geq 0} \sum_{k=0}^n \int_u \omega(Y_0, Y_1)^k \int_{u'} \omega(\bar{v} Y_0, \bar{v} Y_1)^{n-k} \Big|_{Y_j = (\bar{v}' \circ \bar{v})^{-1} X_j : j=0,1} \\ &= F_v(X_0, X_1)^{v'} F_{v'}(X_0, X_1). \end{aligned}$$

\square

Corollary 4.9. *$\text{Li}(z, X_0, X_1)$ is quasi-modular with respect to $PSL(2, \mathbb{Z})$.*

Proof. This is immediate from Theorems 4.6 and 4.8. \square

4.3. Monodromy as modularity. By definition of the $PSL(2, \mathbb{Z})$ action and the fact that $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{01})$ is contained in the kernel of $[\cdot]$, it is evident that the restriction of the $PSL(2, \mathbb{Z})$ action on $\text{Li}(z)$ to the subgroup $\Gamma(2)/\{\pm I\}$ isomorphic to $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{01})$, is one and the same as the monodromy action. In other words, the monodromy of $\text{Li}(z, X_0, X_1)$ is encoded in quasi-modularity statements. More precisely, identifying any $g \in \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \overrightarrow{01})$ with $\gamma \in PSL(2, \mathbb{Z})$ as described in Remark 3.11, the monodromy of $\text{Li}(z, X_0, X_1)$ about g is equal to $\text{Li}^\gamma(z, X_0, X_1)$. As a consequence of 4.6 and 4.8, determining the monodromy is now an easy calculation. For example, about the generators of the fundamental group, as first proven in [MPvdH00] by means of direct methods, we have

Proposition 4.10. *The monodromy of $\text{Li}(z, X_0, X_1)$ about the loop r^2 about 0 in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ based at $\overrightarrow{01}$ is given by*

$$\text{Li}^{\rho^2}(z, X_0, X_1) = \exp(2i\pi X_0) \text{Li}(z, X_0, X_1),$$

while that about the loop sr^2s about 1 in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ is given by

$$\text{Li}^{\sigma\rho^2\sigma}(z, X_0, X_1) = \Phi_{KZ}(X_0, X_1)^\sigma \exp(-2\pi i X_1) \Phi_{KZ}(X_0, X_1) \text{Li}(z, X_0, X_1).$$

Proof. Recall that the loop r^2 about 0 in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ based at $\overrightarrow{01}$ corresponds to ρ^2 in $PSL(2, \mathbb{Z})$. Now

$$\begin{aligned} \text{Li}^{\rho^2}(z, X_0, X_1) &= F_\rho(X_0, X_1)^\rho F_\rho(X_0, X_1) \text{Li}(z, X_0, X_1) \\ &= \exp(\pi i X_0)^\rho \exp(\pi i X_0) \text{Li}(z, X_0, X_1) \\ &= \exp(2\pi i X_0) \text{Li}(z, X_0, X_1) \end{aligned}$$

since $\bar{\rho}(X_0) = X_0$.

The loop about 1 in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ based at $\overrightarrow{01}$ is sr^2s in former notation, corresponding to $\sigma\rho^2\sigma$ in $PSL(2, \mathbb{Z})$.

$$\begin{aligned} \text{Li}^{\sigma\rho^2\sigma}(z, X_0, X_1) &= F_\sigma(X_0, X_1)^{\sigma\rho^2} F_\rho(X_0, X_1)^{\sigma\rho} F_\rho(X_0, X_1)^\sigma F_\sigma(X_0, X_1) \text{Li}(z, X_0, X_1) \\ &= \Phi_{KZ}(X_0, X_1) \exp(-\pi i X_1) \exp(-\pi i X_1) \Phi_{KZ}(X_1, X_0)^\sigma \text{Li}(z, X_0, X_1) \\ &\quad \text{from the definition of the respective actions of } \bar{\sigma} \text{ and } \bar{\rho} \text{ on } X_0, X_1. \end{aligned}$$

□

The method of proof gives a very flexible means of determining the monodromy along any path.

4.4. The power series realization of $PSL(2, \mathbb{Z})$.

Theorem 4.11. *The mapping $PSL(2, \mathbb{Z}) \rightarrow \mathbb{C} \langle\langle X_0, X_1 \rangle\rangle$ given by $\alpha \mapsto F_\alpha(X_0, X_1)$ is injective.*

Proof. Suppose to the contrary that there exists some non-trivial $\alpha \in PSL(2, \mathbb{Z})$ for which $F_\alpha(X_0, X_1) = 1$. Then also $F_\alpha(\bar{\alpha}X_0, \bar{\alpha}X_1) = 1$, since $\bar{\alpha}$ is invertible. But then

$$\int_{\Psi^{-1}\alpha} \omega(X_0, X_1)^n = 0$$

for each $n \geq 1$, since each such integral expression is homogeneous of degree n in the X_j .

The coefficients of the monomials $X_{i_1} \dots X_{i_n}$ here are all of the form of

$$\int_{\Psi^{-1}\alpha} \kappa_{i_1} \dots \kappa_{i_n}$$

where κ_{i_j} is either $\kappa_0 := \frac{dz}{z}$ or $\kappa_1 := \frac{dz}{1-z}$. Hence each such integral is zero. But then by CHEN'S π_1 DE RHAM Theorem (given for this case in [Hai]), necessarily $\Psi^{-1}\alpha$ (and hence α itself) is trivial - a contradiction. \square

Let Γ denote an arbitrary fixed subgroup of $PSL(2, \mathbb{Z})$ and define

$$\mathcal{F}_\Gamma := \{F_\alpha(X_0, X_1) \in \mathbb{C} \langle\langle X_0, X_1 \rangle\rangle \mid \alpha \in \Gamma\}.$$

Lemma 4.12. *The elements of $\mathcal{F}_{PSL(2, \mathbb{Z})}$ are group-like.*

Proof. $\Phi_{KZ}(X_0, X_1)$ is group-like by construction. $e^{i\pi X_0}$ is group-like since X_0 is primitive. In fact, replacing (X_0, X_1) in each of these formal series by any pair of primitive elements of $\mathbb{C} \langle X_0, X_1 \rangle$, the resulting series are also group-like. Now the images of X_0 and X_1 under the action of the elements of $SL(2, \mathbb{Z}/2\mathbb{Z})$ are all primitive. Consequently, each $F_\alpha(X_0, X_1)$ is a product of group-like elements, making it group-like too, since the LIE exponentials form a group. \square

Endow \mathcal{F}_Γ with a multiplication \otimes coming from the $SL(2, \mathbb{Z}/2\mathbb{Z})$ action - i.e. set

$$F_\beta(X_0, X_1) \otimes F_\alpha(X_0, X_1) := F_\alpha(X_0, X_1)^\beta F_\beta(X_0, X_1) = F_{\beta \circ \alpha}(X_0, X_1).$$

This is well-defined by 4.11.

Then from 4.11 and 4.8 one obtains

Theorem 4.13. *$(\mathcal{F}_\Gamma, \otimes)$ is a group which is isomorphic to (Γ, \circ) .*

5. THE $PSL(2, \mathbb{Z})$ 1-COCYCLE ON $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \mathcal{C})$

MINHYONG KIM suggested to the author a context in which the $PSL(2, \mathbb{Z})$ 1-cocycle studied above ought to be seen to arise naturally, namely as the $PSL(2, \mathbb{Z})$ action on the (pro)unipotent fundamental group of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ at the canonical basepoint \mathcal{C} (see §1.3 above) coming from the embedding of $PSL(2, \mathbb{Z})$ into $PGL(2, \mathbb{C})$, the space of automorphisms of the space (i.e. \mathbb{P}^1) underlying the DELIGNE canonical extensions of the unipotent bundles on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. Although this viewpoint has so far not yielded a new proof of the main result of the paper, endowing as it does the power series realization of $PSL(2, \mathbb{Z})$ with geometric meaning, it is certainly a natural perspective. With this in mind, here an alternate approach to defining a $PSL(2, \mathbb{Z})$ action on $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \mathcal{C})$ is demonstrated, which comes directly from the previous sections.

An arbitrary $(\mathcal{V}, \nabla') \in \text{Ob}(\mathbf{Un}(\mathbb{P}^1 \setminus \{0, 1, \infty\}))$ is isomorphic to

$$(\mathcal{O}_{\mathbb{P}^1 \setminus \{0, 1, \infty\}}^r, d - N_0 \frac{dz}{z} - N_1 \frac{dz}{1-z})$$

where r is some integer and N_0, N_1 are nilpotent matrices (see Proposition 1.4). By the nilpotence of the N_j , only finitely many of the expressions $N_{j_1} \dots N_{j_k}$ for $j_l \in \{0, 1\}$ are non-zero. Thus, we can formally substitute N_0 and N_1 in an arbitrary local section $L_a(z, X_0, X_1)$ of \mathcal{U} , say $L_a(z, X_0, X_1) \in \Gamma(U_a, \mathcal{U})$ as in 4.1 above, and obtain a local section of (\mathcal{V}, ∇') in $\Gamma(U_a, \mathcal{V})$ which comprises a finite number of terms and for which we write $L_a(z, N_0, N_1)$. Then a $PSL(2, \mathbb{Z})$ action is induced on $L_a(z, N_0, N_1)$ by that on $L_a(z, X_0, X_1)$. We shall write $L_a^\alpha(z, N_0, N_1)$ for the action of $\alpha \in PSL(2, \mathbb{Z})$ on $L_a(z, N_0, N_1)$.

Now choosing a lifting of all local flat sections of all unipotent (\mathcal{V}, ∇') defined near tangential basepoint \overrightarrow{ab} to the DELIGNE canonical extension, say $(\tilde{\mathcal{V}}, \tilde{\nabla}')$, is in other language the same as picking a path from \overrightarrow{ab} to the canonical basepoint \mathcal{C} , (see §1.3). Fixing such a choice of path, the $PSL(2, \mathbb{Z})$ action on sections of (\mathcal{V}, ∇') as described above then lifts to an action on the global sections of $(\tilde{\mathcal{V}}, \tilde{\nabla}')$. Explicitly, this is done as follows:

Using the universal property of \mathcal{U} as above, to give such a path it suffices to describe the lift of the polylogarithm generating series $\text{Li}(z, X_0, X_1)$ as a section of \mathcal{U} , to the canonical extension $\tilde{\mathcal{U}}$. Such a path is given by lifting $\text{Li}(z, X_0, X_1)$ to the unique flat section with local description near $0 \in \mathbb{P}^1$ given by

$$z^{-X_0} \text{Li}(z, X_0, X_1)$$

(see §1.3 - this is the usual DELIGNE canonical extension near 0). A simple calculation using Proposition 4.10 confirms that this local section is single valued in some neighbourhood of 0. Once and for all fix this as the path from $\overrightarrow{01}$ to \mathcal{C} used in subsequent constructions.

Now define the action of any given $\alpha \in PSL(2, \mathbb{Z})$ on the section of $\tilde{\mathcal{U}}$ which is the unique flat global section given near 0 by $z^{-X_0} \text{Li}(z, X_0, X_1)$, as the unique flat global section given near $\bar{\alpha}z$ by

$$(\bar{\alpha}z)^{-\bar{\alpha}^{-1}X_0} \text{Li}^\alpha(z, X_0, X_1).$$

As it should, the action of σ factors through that of $\bar{\sigma}$. Indeed, notice that $z^{-X_0} \text{Li}(z, X_0, X_1)$ acted upon by σ is the *same* as

$$(\bar{\sigma}z)^{-\bar{\sigma}^{-1}X_0} \text{Li}(\bar{\sigma}z, \bar{\sigma}^{-1}X_0, \bar{\sigma}^{-1}X_1).$$

Again by universality of \mathcal{U} , also using the fact that the polylogarithm generating series forms a basis of flat sections of \mathcal{U} , one sees that this action determines a tensor compatible family of maps of the global sections of the DELIGNE canonical extensions of the unipotent bundles on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, and hence an element of $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}, \mathcal{C})$. In this way, $PSL(2, \mathbb{Z})$ acts on the fundamental group via both a left and a right action, by post- and pre-composition respectively, in each of which a 1-cocycle on $\mathbb{C} \ll X_0, X_1 \gg_\Lambda$ arises as before (cf. Theorem 4.8).

6. $PSL(2, \mathbb{Z})$ AND THE QUASI-TRIANGULAR QUASI-HOPF ALGEBRAS

6.1. A pair of $PSL(2, \mathbb{Z})$ -torsors and the DRINFEL'D associator.

Using the power series realization given above, we proceed to exhibit two disjoint $PSL(2, \mathbb{Z})$ -torsors comprising sections of \mathcal{P} . The guiding philosophy here is that the formal power series DRINFEL'D associator Φ_{KZ} should not satisfy relations other than the hexagonal relations and

$$(21) \quad \Phi_{KZ}(Z_0, Z_1)^{-1} = \Phi_{KZ}(-Z_1, -Z_0)$$

for any formal non-commuting variables Z_0 and Z_1 . (Ignoring the extra braid relation in [Dri91].) Indeed, to attain the results of this section, it is necessary to show that among certain expressions constructed from the R -matrix $\exp(i\pi X_0)$ and Φ_{KZ} itself, no other relations arise.

For any formal power series $E(X_0, X_1)$ and any subgroup Γ of $PSL(2, \mathbb{Z})$, now define $\mathcal{E}_{E, \Gamma}$ to be the space of global sections of \mathcal{U} given by

$$\{E(X_0, X_1)^\alpha F_\alpha(X_0, X_1) \text{Li}(z, X_0, X_1) \in \Gamma(\mathcal{U}, \mathbb{P}^1 \setminus \{0, 1, \infty\}) | \alpha \in \Gamma\}.$$

When E is group-like, $\mathcal{E}_{E,PSL(2,\mathbb{Z})}$ is contained in \mathcal{P} by Lemma 4.12. A distinguished space of this kind is that for which $E(X_0, X_1) = 1$, as one sees by combining the fact that

$$\mathcal{E}_{1,PSL(2,\mathbb{Z})} = \mathcal{E}_{F_\beta,PSL(2,\mathbb{Z})}$$

for any $\beta \in PSL(2, \mathbb{Z})$ with the following immediate consequence of 4.13:

Corollary 6.1. *For any subgroup Γ of $PSL(2, \mathbb{Z})$, the set $\mathcal{E}_{1,\Gamma}$ of global sections of \mathcal{P} is a Γ -torsor over $\mathbb{P}^1 \setminus \{0, 1, \infty\}$.*

We would like to know for which other group-like power series E the space $\mathcal{E}_{E,\Gamma}$ is a Γ -torsor, particularly when $\Gamma = PSL(2, \mathbb{Z})$. A related question is that of determining which such E give rise to distinct $PSL(2, \mathbb{Z})$ -torsors. In less vague form: can one explicitly characterise the quotient of the group-like elements of $\mathbb{C} \ll X_0, X_1 \gg$ by $\mathcal{F}_{PSL(2,\mathbb{Z})} \simeq PSL(2, \mathbb{Z})$? In such generality, the answer is not apparent to the author. However, in one special case, a $PSL(2, \mathbb{Z})$ -torsor different to $\mathcal{E}_{1,PSL(2,\mathbb{Z})}$ can be identified, namely taking $E(X_0, X_1) = \Phi_{KZ}(X_0, X_1)$. Proving this relies on the

Lemma 6.2. *For any $\eta \in PSL(2, \mathbb{Z})$:*

- (a) $\Phi_{KZ}(X_0, X_1)^\eta$ has no linear terms (i.e. no terms in X_0 and X_1 alone).
- (b) The terms of degree 2 in $\Phi_{KZ}(X_0, X_1)^\eta$ are

$$\text{sgn}(\bar{\eta})\zeta(2)(X_1X_0 - X_0X_1)$$

where $\text{sgn}(\bar{\eta})$ denotes the sign of the permutation $\bar{\eta} \in S_3$.

Proof. For $\bar{\eta} = 1$, (a) is a fundamental, well-known fact - cf. [Car01]. Since $\bar{\eta}X_j$ is linear in X_0 and X_1 with no constant term for both $j = 0$ and $j = 1$, (a) is immediate in the general case.

For $\bar{\eta} = 1$, (b) is also well-known - cf. [LM96]. Then one computes

$$\zeta(2)(X_1X_0 - X_0X_1)^\eta$$

directly for each class of $\bar{\eta}$ in $SL(2, \mathbb{Z}/2\mathbb{Z}) \setminus \{1\}$, and sees that for $\bar{\eta} = \bar{\sigma} \circ \bar{\rho}$ and $\bar{\rho} \circ \bar{\sigma}$ the expression is invariant under the η action, whereas in the remaining three cases the η action reverses the sign. \square

Theorem 6.3. *If η is an element of $PSL(2, \mathbb{Z})$ for which $\bar{\eta}$ is an even permutation, then there is no $\alpha \in PSL(2, \mathbb{Z})$ for which*

$$\text{Li}^\alpha(z, X_0, X_1) = \Phi_{KZ}(X_0, X_1)^\eta \text{Li}(z, X_0, X_1).$$

Proof. Suppose contrary to the assertion that there exists some $\alpha \in PSL(2, \mathbb{Z})$ for which

$$\text{Li}^\alpha(z, X_0, X_1) = \Phi_{KZ}(X_0, X_1)^\eta \text{Li}(z, X_0, X_1).$$

The proof is carried out by ruling out possibilities for the congruence class of α modulo $SL(2, \mathbb{Z}/2\mathbb{Z})$:

Firstly, $\bar{\alpha}$ is not trivial: If this were not so, α would be given by some expression of the form of

$$g(\rho^2, \sigma \circ \rho^2 \circ \sigma)$$

where $g(x, y)$ denotes some element of the free group on the two letters x and y . But then $F_\alpha(X_0, X_1) = \Phi_{KZ}(X_0, X_1)^\eta$ would be expressible as $\Phi_{KZ}(X_0, X_1)^\eta = g(\exp(2\pi i X_0), \Phi_{KZ}(X_0, X_1) \exp(-2\pi i X_1) \Phi_{KZ}(X_0, X_1)^\sigma)$.

On the right hand side, the coefficient of $X_1 X_0$ coming from the associators Φ_{KZ} and Φ_{KZ}^σ add to zero by 6.2, since $\bar{\sigma}$ is odd. Hence, the $X_1 X_0$ term on the right side has coefficient of the form of $(2\pi i)^2 N$ for some integer N . But in Φ_{KZ}^η , the coefficient of $X_1 X_0$ is of the form of $\text{sgn}(\bar{\eta})\zeta(2) = \pm \frac{\pi^2}{6}$, a contradiction (regardless of the parity of $\bar{\eta}$).

Next $\bar{\alpha} \neq \bar{\sigma}$: Should this be false, α would be of the form of

$$g_0(\rho^2, \sigma \circ \rho^2 \circ \sigma) \circ \sigma \circ g_1(\rho^2, \sigma \circ \rho^2 \circ \sigma)$$

where $g_0(x, y)$ and $g_1(x, y)$ are again elements of the free group on x and y . Since the reduction modulo $SL(2, \mathbb{Z}/2\mathbb{Z})$ of each expression of the form of $g_j(\rho^2, \sigma \circ \rho^2 \circ \sigma)$ is trivial, this decomposition of α would give

$$\begin{aligned} \Phi_{KZ}(X_0, X_1)^\eta &= g_1(\exp(-2\pi i X_1), \Phi_{KZ}^\sigma \exp(2\pi i X_0) \Phi_{KZ}) \Phi_{KZ}(X_0, X_1)^\sigma \\ &\quad \cdot g_0(\exp(2\pi i X_0), \Phi_{KZ} \exp(-2\pi i X_1) \Phi_{KZ}^\sigma). \end{aligned}$$

But the $X_1 X_0$ coefficients on both sides cannot agree when $\bar{\eta}$ is even: On the left side, this coefficient is $\text{sgn}(\bar{\eta})\zeta(2)$ and on the right, $-\zeta(2) + (2\pi i)^2 M$ where M is some integer.

The remaining cases are dealt with by similar means, instead considering only the linear terms. We expound this method completely only in the most complicated situation: Suppose that $\bar{\alpha} = \bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma}$. Then for $j = 0, 1, 2, 3$ there exist elements $g_j(x, y)$ of the free group on $\{x, y\}$, for which α is one of the expressions

$$g_0(\rho^2, \sigma \rho^2 \sigma) \circ \sigma \circ g_1(\rho^2, \sigma \rho^2 \sigma) \circ \rho^{\pm 1} \circ g_2(\rho^2, \sigma \rho^2 \sigma) \circ \sigma \circ g_3(\rho^2, \sigma \rho^2 \sigma),$$

either by (12) or the topological picture of §3, (writing $\sigma \rho^2 \sigma$ for $\sigma \circ \rho^2 \circ \sigma$). Again because the reduction modulo $SL(2, \mathbb{Z}/2\mathbb{Z})$ of each

expression of the form of $g_j(\rho^2, \sigma \circ \rho^2 \circ \sigma)$ is trivial, it follows from the action of α on $\text{Li}(z, X_0, X_1)$ by means of the above expressions that

$$(22) \quad \begin{aligned} \Phi_{KZ}(X_0, X_1)^\eta &= G_3(X_0, X_1)^{\sigma \circ \rho \circ \sigma} \Phi_{KZ}(-X_1, -X_0)^{\sigma \circ \rho} G_2(X_0, X_1)^{\sigma \circ \rho} \\ &\quad \cdot e^{\mp i\pi X_1} G_1(X_0, X_1)^\sigma \Phi_{KZ}(-X_1, -X_0) G_0(X_0, X_1), \end{aligned}$$

writing $g_j(\exp(2\pi i X_0), \Phi_{KZ} \exp(-2\pi i X_1) \Phi_{KZ}^\sigma) = G_j(X_0, X_1)$ for each $j = 0, 1, 2, 3$. Now on the right hand side of this supposed expansion of $\Phi_{KZ}(X_0, X_1)^\eta$, the linear term is of the form of $\mp i\pi X_1 + 2\pi i(a_0 X_0 + a_1 X_1)$ where a_0 and a_1 are integers. This term does not vanish. On the other hand, by Lemma 6.2 (a) $\Phi_{KZ}(X_0, X_1)^\eta$ has no linear terms. This is a contradiction.

The other three cases ($\bar{\alpha}$ being respectively $\bar{\rho}$, $\bar{\rho} \circ \bar{\sigma}$ or $\bar{\sigma} \circ \bar{\rho}$) are similar. \square

Theorem 6.3 may also be stated as follows:

Corollary 6.4. *If η is a fixed element of $PSL(2, \mathbb{Z})$ for which $\bar{\eta}$ is even, then the spaces of sections $\mathcal{E}_{\Phi_{KZ}, PSL(2, \mathbb{Z})}^\eta$ and $\mathcal{E}_{1, PSL(2, \mathbb{Z})}$ are disjoint.*

Proof. Suppose that there exist some $\alpha, \beta \in PSL(2, \mathbb{Z})$ for which

$$\Phi_{KZ}(X_0, X_1)^{\alpha \circ \eta} F_\alpha(X_0, X_1) = F_\beta(X_0, X_1).$$

Then since $F_\alpha^{\alpha^{-1}} F_{\alpha^{-1}} = 1$, also $F_\alpha F_{\alpha^{-1}}^\alpha = 1$, so

$$\Phi_{KZ}(X_0, X_1)^{\alpha \circ \eta} = F_\beta(X_0, X_1) F_{\alpha^{-1}}(X_0, X_1)^\alpha$$

and hence

$$\Phi_{KZ}(X_0, X_1)^\eta = F_\beta(X_0, X_1)^{\alpha^{-1}} F_{\alpha^{-1}}(X_0, X_1) = F_{\alpha^{-1} \circ \beta}(X_0, X_1)$$

violating Theorem 6.3. \square

Lemma 6.5. *If E is an invertible formal power series, and $E^\alpha F_\alpha = E^\beta F_\beta$ for some α, β in $PSL(2, \mathbb{Z})$, then $E = E^\gamma F_\gamma$ where γ has order 2 or 3.*

Proof. Assuming $E^\alpha F_\alpha = E^\beta F_\beta$, then

$$E^{\alpha^{-1} \circ \alpha} F_\alpha^{\alpha^{-1}} = E^{\alpha^{-1} \circ \beta} F_\beta^{\alpha^{-1}}.$$

Now $F_\alpha^{\alpha^{-1}} F_{\alpha^{-1}} = 1$, so

$$E = E^{\alpha^{-1} \circ \beta} F_\beta^{\alpha^{-1}} F_{\alpha^{-1}} = E^{\alpha^{-1} \circ \beta} F_{\alpha^{-1} \circ \beta}$$

and we take $\gamma = \alpha^{-1} \circ \beta$.

But then

$$E = E^\gamma F_\gamma = (E^\gamma F_\gamma)^\gamma F_\gamma = E^{\gamma^2} F_{\gamma^2} = \dots = E^{\gamma^k} F_{\gamma^k}$$

for any $k \geq 1$. Now $\bar{\gamma}$ has order 2 or 3, being an element of S_3 . Hence $E = EF_{\gamma^k}$ where $k = 2$ or $k = 3$. Making use of the invertibility of E , the assertion follows by application of 4.11. \square

Theorem 6.6. *For any $\bar{\eta} \in SL(2, \mathbb{Z}/2\mathbb{Z})$ and any lift η of $\bar{\eta}$ to $PSL(2, \mathbb{Z})$, there are no distinct α and β in $PSL(2, \mathbb{Z})$ for which*

$$\Phi_{KZ}^{\alpha\eta} F_\alpha = \Phi_{KZ}^{\beta\eta} F_\beta.$$

Proof. The case of $\bar{\eta} = \bar{\sigma}$ is covered by Theorem 4.11, since

$$\Phi_{KZ}^{\alpha\sigma} F_\alpha = F_\sigma^\alpha F_\alpha = F_{\alpha\sigma}.$$

The remaining proofs run along the same pattern to each other, so we show only that for $\bar{\eta} = 1$:

Suppose instead that there exist some α and β in $PSL(2, \mathbb{Z})$ for which

$$\Phi_{KZ}^\alpha F_\alpha = \Phi_{KZ}^\beta F_\beta.$$

Then by the Lemma 6.5, there exists some γ of order 2 or 3 in $PSL(2, \mathbb{Z})$, for which

$$(23) \quad \Phi_{KZ} = \Phi_{KZ}^\gamma F_\gamma.$$

Firstly suppose that γ has order 2. Then necessarily $\bar{\gamma} = \bar{\sigma}$. Consequently,

$$\Phi_{KZ} = \Phi_{KZ}^\sigma F_\gamma$$

so that

$$\Phi_{KZ}^2 = F_\gamma.$$

It now follows that $\gamma \neq \sigma$, since, were this to be the case, Φ_{KZ}^2 would have to equal $F_\sigma = \Phi_{KZ}^\sigma$, but by means of 6.2, an examination of the coefficients of the $X_1 X_0$ term of these respective power series yields $2\zeta(2)$ for the first and $-\zeta(2)$ for the second, an impossibility.

Again because $\bar{\gamma} = \bar{\sigma}$, as in the proof of 6.3, we have

$$\gamma = g_0(\rho^2, \sigma\rho^2\sigma) \circ \sigma \circ g_1(\rho^2, \sigma\rho^2\sigma),$$

where for $j = 0, 1$, $g_j(x, y)$ is some word in x, y, x^{-1} and y^{-1} . At the same time, since γ has order 2, one sees that $g_0 = g_1^{-1}$. But then

$$\begin{aligned} \Phi_{KZ}^2 &= g_1(\exp(2\pi i X_0), \Phi_{KZ} \exp(-2\pi i X_1) \Phi_{KZ}^\sigma)^\sigma \\ &\quad \Phi_{KZ}^\sigma \cdot g_1^{-1}(\exp(2\pi i X_0), \Phi_{KZ} \exp(-2\pi i X_1) \Phi_{KZ}^\sigma) \\ (24) \quad &= g_1(\exp(-2\pi i X_1), \Phi_{KZ}^\sigma \exp(2\pi i X_0) \Phi_{KZ}). \end{aligned}$$

$$(25) \quad \Phi_{KZ}^\sigma \cdot g_1^{-1}(\exp(2\pi i X_0), \Phi_{KZ} \exp(-2\pi i X_1) \Phi_{KZ}^\sigma).$$

Comparing the $X_1 X_0$ coefficients of both sides produces a contradiction: Indeed, on the left side this coefficient is $2\zeta(2)$ by 6.2. On the

other hand, on the right the coefficient is of the form of $\zeta(2)A + (2\pi i)^2 B$ where A and B are integers and the value of A can be computed using 6.2: As before, for any $\delta \in PSL(2, \mathbb{Z})$ the $X_1 X_0$ terms in each expression of the form of $(\Phi_{KZ} \exp(-2\pi i X_1) \Phi_{KZ}^\sigma)^\delta$ are the negatives of each other (again by 6.2, since $\bar{\sigma}$ has odd parity as an element of S_3). Hence the only contribution to A comes from the Φ_{KZ}^σ factor of F_γ - i.e. $A = -1$. Since B is to be an integer for which

$$-\zeta(2) + (2\pi i)^2 B = 2\zeta(2) = \frac{\pi^2}{3},$$

this is impossible.

We conclude that if $\Phi_{KZ} = \Phi_{KZ}^\gamma F_\gamma$, then γ must have order 3. In this case, $\bar{\gamma} = \bar{\sigma} \circ \bar{\rho}$ or $\bar{\gamma} = \bar{\rho} \circ \bar{\sigma}$. In the first case, by (23) and the fact that $\Phi_{KZ}^{-1} = \Phi_{KZ}^\sigma$, one has

$$(26) \quad \Phi_{KZ}^\rho \Phi_{KZ} = F_\gamma$$

for some $\gamma \in PSL(2, \mathbb{Z})$. By similar arguments to those above, F_γ is given by

$$\begin{aligned} & h_1^{-1}(\exp(2\pi i X_0), \Phi_{KZ}(X_0, X_1) \exp(-2\pi i X_1) \Phi_{KZ}(X_0, X_1)^\sigma)^{\sigma \circ \rho} \exp(-\pi i X_1) \\ & h_2(\exp(2\pi i X_0), \Phi_{KZ}(X_0, X_1) \exp(-2\pi i X_1) \Phi_{KZ}(X_0, X_1)^\sigma)^\sigma \\ & \Phi_{KZ}(X_0, X_1)^\sigma h_1(\exp(2\pi i X_0), \Phi_{KZ}(X_0, X_1) \exp(-2\pi i X_1) \Phi_{KZ}(X_0, X_1)^\sigma) \end{aligned}$$

where $h_j(x, y)$ is a word in the symbols $x^{\pm 1}, y^{\pm 1}$, for both $j = 1$ and 2 . If this expression is to equal $\Phi_{KZ}^\rho \Phi_{KZ}$, the $X_1 X_0$ terms of both sides of (26) must agree. However, the coefficient of this term in the product of associators is 0, by 6.2, while in the term coming from the expansion of γ , the coefficient is of the form of $\zeta(2)C + (\pi i)^2 D$, for some integers C and D , as before. Exactly as above, one sees that necessarily $C = -1$, which is absurd.

Finally, should $\bar{\gamma} = \bar{\rho} \circ \bar{\sigma}$, a similar proof goes through as before: One finds that the equality

$$\Phi_{KZ}^{\sigma \circ \rho \circ \sigma} \Phi_{KZ} = F_\gamma$$

would hold. By the same type of argument as above, computing the form of F_γ and the coefficient of $X_1 X_0$ on the respective sides of the equation, one arrives at

$$0 = \zeta(2) + (\pi i)^2 M$$

for integer M , an impossibility. (Here the $+\zeta(2)$ on the right comes from the coefficient of $X_1 X_0$ in $\Phi_{KZ}^{\rho \circ \sigma}$.) \square

Now for each class $\bar{\eta} \in SL(2, \mathbb{Z}/2\mathbb{Z})$ with $\eta \in PSL(2, \mathbb{Z})$ some lift of $\bar{\eta}$, define

$$\mathcal{F}_{\Phi\eta, PSL} := \{\Phi_{KZ}^{\alpha\eta}(X_0, X_1)F_\alpha(X_0, X_1) \in \mathbb{C} \ll X_0, X_1 \gg \mid \alpha \in PSL(2, \mathbb{Z})\}.$$

Of course, $\mathcal{F}_{\Phi\eta, PSL} = \mathcal{F}_{\Phi v, PSL}$ for any $v \in PSL(2, \mathbb{Z})$ with $\bar{v} = \bar{\eta}$.

Now set

$$\Phi_{KZ}^{\beta\circ\eta}F_\beta \odot \Phi_{KZ}^{\alpha\eta}F_\alpha := \Phi_{KZ}^{\beta\circ\alpha\circ\eta}(F_\beta \circledast F_\alpha) = \Phi_{KZ}^{\beta\circ\alpha\circ\eta}F_{\beta\circ\alpha}.$$

By the above theorem \odot gives a well-defined mapping of $\mathcal{F}_{\Phi\eta, PSL} \times \mathcal{F}_{\Phi\eta, PSL}$ into $\mathcal{F}_{\Phi\eta, PSL}$. Also, we can define an action of $PSL(2, \mathbb{Z})$ on $\mathcal{F}_{\Phi\eta, PSL}$ by setting

$$\gamma \star \Phi_{KZ}^{\alpha\eta}F_\alpha = \Phi_{KZ}^{\gamma\circ\alpha\circ\eta}F_{\gamma\circ\alpha}.$$

With this action,

Corollary 6.7. *For every $\bar{\eta} \in SL(2, \mathbb{Z}/2\mathbb{Z})$ and any lift thereof to $\eta \in PSL(2, \mathbb{Z})$, $\mathcal{F}_{\Phi\eta, PSL(2, \mathbb{Z})}$ (and hence also $\mathcal{E}_{\Phi\eta, PSL(2, \mathbb{Z})}$) is a $PSL(2, \mathbb{Z})$ -torsor.*

Proof. The action of $PSL(2, \mathbb{Z})$ is faithful by Theorem 6.6. □

By 6.4, we have produced at least two disjoint $PSL(2, \mathbb{Z})$ -torsors.

Remark 6.8. The fact that Φ_{KZ} is not of the form of F_α for any $\alpha \in PSL(2, \mathbb{Z})$ (by 6.3) aligns with the expectation that no relations similar in structure to the hexagonal relations (besides these relations themselves) link the associator to admissible products of the R -matrix with Φ_{KZ} under the associated $SL(2, \mathbb{Z}/2\mathbb{Z})$ -action. On the other hand, Theorem 6.6 limits the relations of the type of (21), and one expects that more generally, no other such relations exist.

6.2. Mapping $PSL(2, \mathbb{Z})$ into qtqH algebras. The power series realization of $PSL(2, \mathbb{Z})$ gives an embedding of $PSL(2, \mathbb{Z})$ into the formal model of quasi-triangular quasi-HOPF algebras given by DRINFELD - i.e., the formal power series algebra $\mathbb{C} \ll X_0, X_1 \gg$ with distinguished elements $\Phi_{KZ}(X_0, X_1)$ and $R = \exp(i\pi X_0)$. In this context, the hexagonal relations reflect the hexagonal axioms given in §1.4, which dictate how the associator and R -matrix interact in a general qtqH algebra.

Suppose that \mathfrak{g} is a LIE algebra over \mathbb{C} and that $t \in \mathfrak{g} \otimes \mathfrak{g}$ is symmetric and \mathfrak{g} -invariant. Then form the universal enveloping algebra $U(\mathfrak{g})$ and write $A = U(\mathfrak{g})[[h]]$. Situations of geometric interest arise when \mathfrak{g} is the LIE algebra of the unipotent completion of some fundamental

group $\pi_1^{\text{un}}(X, c)$: See [Kim09] for a general construction of the universal prounipotent pro-bundle with connection on a scheme X using $U(\text{Lie}(\pi_1^{\text{un}}(X, c)))$.

DRINFEL'D showed in [Dri91] that A can be endowed with the structure of quasi-triangular quasi-HOPF algebra by taking the associator to be

$$\Phi = \Phi_{KZ}(\hbar t^{12}, -\hbar t^{23}) \in A \otimes A \otimes A$$

where \hbar denotes PLANCK'S constant $\hbar = h/2\pi i$, with $t^{12} = t \otimes 1$ and $t^{23} = 1 \otimes t$; and the R -matrix $R = \exp(i\pi\hbar t)$. (In our version of DRINFEL'D'S formal model, we take $h = 2\pi i$.)

This provides motivation for the following set-up: Let k be an arbitrary field of characteristic 0, and $A = U(\mathfrak{g})[[\hbar]]$ as above. In this general setting, DRINFEL'D (loc. cit.) proved that one can form a qtqH algebra $(A, \varepsilon, \Delta, \Phi, R)$ which by means of some gauge transformation if necessary, can be assumed to have the symmetry properties: $R^{21} = R$ and $\Phi^{321} = \Phi^{-1}$, where if $R = \sum a_i \otimes b_i$, then $R^{21} = \sum b_i \otimes a_i$, and for $\Phi = \sum x_i \otimes y_i \otimes z_i$, then $\Phi^{321} = \sum z_i \otimes y_i \otimes x_i$. These last expressions can be described via the action of the elements $(1 \ 2)$ of S_2 and $(1 \ 3)$ of S_3 respectively. Defining $\tilde{R} = 1 \otimes R$, then by the symmetry, S_3/S_2 acts on \tilde{R} . This is in line with the action of S_3 on the single formal variable X_0 - see the table in §2 - when we take the generator of S_2 embedded into S_3 to be $\bar{\rho} = (2 \ 3)$.

To be consistent with the approach taken in this paper, the action of $\bar{\sigma}$ on Φ ought to give Φ^{-1} . For this to be the case, we must also take $\bar{\sigma} = (1 \ 3)$.

Then defining \tilde{R}^{ijk} and Φ^{ijk} as in §1.4 above, and the action of $\bar{\lambda} \in S_3$ on \tilde{R} by $\tilde{R}^{\bar{\lambda}}$, we have

$$\begin{aligned} \tilde{R} &= \tilde{R}^{132} = \tilde{R}^1 = \tilde{R}^{\bar{\rho}} = \sum 1 \otimes a_i \otimes b_i \\ \tilde{R}^{321} &= \tilde{R}^{312} = \tilde{R}^{\bar{\sigma}} = \tilde{R}^{\bar{\sigma}\bar{\rho}} = \sum a_i \otimes b_i \otimes 1 \\ \tilde{R}^{213} &= \tilde{R}^{231} = \tilde{R}^{\bar{\sigma}\bar{\rho}\bar{\sigma}} = \tilde{R}^{\bar{\rho}\bar{\sigma}} = \sum a_i \otimes 1 \otimes b_i, \end{aligned}$$

and write $\Phi^{321} = \Phi^{\bar{\sigma}}$ and so on. In particular, one finds

$$\begin{aligned} \Phi^{231} &= \Phi^{\bar{\rho}\bar{\sigma}} & \Phi^{312} &= \Phi^{\bar{\sigma}\bar{\rho}} \\ \Phi^{213} &= \Phi^{\bar{\sigma}\bar{\rho}\bar{\sigma}} & \Phi^{132} &= \Phi^{\bar{\rho}}. \end{aligned}$$

In this notation, the hexagonal axioms of (9) and (10) take the form of:

$$(27) \quad (\Delta \otimes \text{id})R = \Phi^{\bar{\sigma}\bar{\rho}} \tilde{R}^{\bar{\rho}\bar{\sigma}} (\Phi^{\bar{\rho}})^{-1} \tilde{R}\Phi = \Phi^{\bar{\sigma}\bar{\rho}} \tilde{R}^{\bar{\rho}\bar{\sigma}} \Phi^{\bar{\rho}\bar{\sigma}} \tilde{R}\Phi$$

and

$$(28) \quad (\text{id} \otimes \Delta)R = (\Phi^{\bar{\rho} \circ \bar{\sigma}})^{-1} \tilde{R}^{\bar{\sigma} \bar{\rho} \bar{\sigma}} \Phi^{\bar{\sigma} \bar{\rho} \bar{\sigma}} \tilde{R}^{\bar{\sigma}} \Phi^{-1} = \Phi^{\bar{\rho}} \tilde{R}^{\bar{\sigma} \bar{\rho} \bar{\sigma}} \Phi^{\bar{\sigma} \bar{\rho} \bar{\sigma}} \tilde{R}^{\bar{\sigma}} \Phi^{\bar{\sigma}}.$$

(Here we use that $(\Phi^{ijk})^{-1} = \Phi^{kji}$.)

Then we can prove:

Theorem 6.9. *If $(A, \varepsilon, \Delta, \Phi, R)$ is a qtqH algebra in which (under a symmetric gauge transformation if necessary) $\Phi^{-1} = \Phi^{321}$ and $R = R^{21}$, and R satisfies*

$$(29) \quad (\text{id} \otimes \Delta)R = \tilde{R}^{-1},$$

then $PSL(2, \mathbb{Z})$ may be represented on $A \otimes A \otimes A$ by the mapping determined by

$$F : \rho \mapsto \tilde{R}$$

and

$$F : \sigma \mapsto \Phi^{\bar{\sigma}},$$

with the $SL(2, \mathbb{Z}/2\mathbb{Z})$ composition rule

$$F(\beta \circ \alpha) = F(\alpha)^{\bar{\beta}} F(\beta).$$

Proof. Since we know that $\Phi^{\bar{\sigma}} = \Phi^{-1}$, it remains only to check that the hexagonal relations are compatible with the relations in $PSL(2, \mathbb{Z})$ and that F preserves all the relations in this group.

Using condition (29) and the relation $\bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma} = \bar{\rho}$ in S_3 , the hexagonal axiom (28) may be expressed as

$$(30) \quad 1 = \tilde{R} \Phi^{\bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma}} \tilde{R}^{\bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma}} \Phi^{\bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma}} \tilde{R}^{\bar{\sigma}} \Phi^{\bar{\sigma}} = F(\sigma \circ \rho \circ \sigma \circ \rho \circ \sigma \circ \rho),$$

so F sends the braid relation in $PSL(2, \mathbb{Z})$ into this hexagonal relation.

Now write $R = \sum_i a_i \otimes b_i$ and $\Delta c_i = \sum_j c_{i,j}^{(1)} \otimes c_{i,j}^{(2)}$ and consider

$$\begin{aligned} [(\Delta \otimes \text{id})R]^{\bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma}} &= \left(\sum_i (\Delta a_i) \otimes b_i \right)^{\bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma}} \\ &= \sum_{i,j} a_{i,j}^{(2)} \otimes a_{i,j}^{(1)} \otimes b_i \\ &= \left(\sum_{i,j} b_i \otimes a_{i,j}^{(1)} \otimes a_{i,j}^{(2)} \right)^{\bar{\sigma}} \\ &= [(\text{id} \otimes \Delta)R]^{\bar{\sigma}}, \end{aligned}$$

exploiting the symmetry $R^{21} = R$ in the last line. Now

$$[(\text{id} \otimes \Delta)R]^{\bar{\sigma}} = [\tilde{R}^{-1}]^{\bar{\sigma}} = [\tilde{R}^{-1}]^{\bar{\sigma} \circ \bar{\rho}}$$

by the hypothesis (29) and the S_3 action on \tilde{R} .

Hence

$$[(\Delta \otimes \text{id})R]^{\bar{\sigma} \circ \bar{\rho} \circ \bar{\sigma}} = [\tilde{R}^{-1}]^{\bar{\sigma} \circ \bar{\rho}}$$

so that

$$[(\Delta \otimes \text{id})R]^{\bar{\sigma}} = \tilde{R}^{-1}.$$

But then the first hexagonal relation (27) is the same as the equation one obtains by applying $\bar{\sigma}$ to both sides of (30). \square

If $(A, \varepsilon, \Delta, \Phi, R)$ is a qtqH algebra satisfying the hypotheses of the theorem, any representation of A induces a representation of $PSL(2, \mathbb{Z})$. Since $\text{Rep}PSL(2, \mathbb{Z})$ is a tannakian category, this does not result in an embedding of monoidal categories of $\text{Rep}A$ into $\text{Rep}PSL(2, \mathbb{Z})$ unless $\text{Rep}A$ is in fact a tensored category. For this to happen, the commutativity isomorphism in $\text{Rep}A$ must be involutory and hence $R^{21} = R^{-1}$. But then in this situation, $R = R^{-1}$, so the representation of $PSL(2, \mathbb{Z})$ on $A \otimes A \otimes A$ factors through $SL(2, \mathbb{Z}/2\mathbb{Z})$!

7. QUASI-MODULARITY IN PROVING THE FUNCTIONAL EQUATION OF $\zeta(s)$

7.1. A topological vision of RIEMANN'S proof. The first of the two proofs of the functional equation satisfied by the RIEMANN zeta function $\zeta(s)$ given by RIEMANN himself in [Rie92] admits a very natural algebro-topological explanation. This is most readily seen by means of the logarithmic co-ordinates on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, for which the analytic continuation is obtained via the contour integral

$$(31) \quad \zeta(s) = \frac{\Gamma(1-s)}{2\pi i} \int_A \frac{z}{1-z} (\log z)^{s-1} \frac{dz}{z},$$

where A denotes a contour moving slightly above the real axis from the vicinity of 0 to some point close to 1, then encircles 1, and returns below the real axis to some point near 0. To make sense of the complex power occurring in this integral, a branch cut for the $\log(\log(\cdot))$ function is required. A suitable choice for the branch cut is exactly the (tangential) path from 0 to 1, which is precisely the path avoided by A as it encloses the point at which $\frac{z}{1-z}$ is singular! Now RIEMANN'S idea was to evaluate the integral on some closed path excluding these singular points - i.e. to make use of CAUCHY'S theorem, which is essentially the topological statement that an integral

$$\int_{\gamma} f(z) dz$$

of a meromorphic f is a functional on homotopy - more precisely on the fundamental group of \mathbb{C} minus the points at which f is singular. To implement this idea, it is necessary to lift A to the RIEMANN surface X on which the logarithm function is single-valued, again marked with a branch cut along the path from 0 to 1 in the principal sheet, making $\log(\log(\cdot))$ single valued. This is the genesis of the contour in \mathbb{C} , which featured in RIEMANN'S original proof.

Evidently it is the branch cut which distinguishes the lift of A to the principal sheet of X from the lifts to other sheets, and which consequently explains the term $-\zeta(s)$ coming from integration in this particular sheet whereas no such term arises from the contributions in other sheets. The harmonic factor $\sin\left(\frac{\pi s}{2}\right)$ in the functional equation comes from the interplay of terms from both sides (above and below) of the $\log(\log(\cdot))$ branch cut, while the $\zeta(1-s)$ term arises from the totality of the residues at lifts of 1 to X , other than in the principal sheet. In these distinct sheets, the values of the logarithm essentially encode monodromy data. In the computation of the residues, the monodromy terms play a vital role.

In a nutshell, RIEMANN'S proof shows that the functional equation for $\zeta(s)$ is a consequence of

$$\frac{\Gamma(1-s)}{2\pi i} \int (\log z)^{s-1} \frac{dz}{1-z}$$

being a homotopy functional - in particular, in some completion of $\pi_1(X \setminus (0,1))$ (omitting the branch cut pertaining to $\log \log(\cdot)$) we evaluate this integral along a path bounding a region on which the integral has no singularities, and the statement that this integral is zero *is* the functional equation.

7.2. Families of integral expressions for $\zeta(s)$. In previous work, [Joy10], the author developed a theory of complex iterated integral generalizing the usual notion of iterated integral as in the work of CHEN. In particular, on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, if $F(z)$ denotes a function with $F(0) = 0$ having TAYLOR series expansion on the unit disc for which the n th coefficient is $O(n^k)$ for some $k \geq 0$, then we define

$$(32) \quad L[F](s, z) = \int_{[0,z]} F(t) \left(\frac{dt}{t} \right)^s := \int_0^z \frac{(\log z - \log t)^{s-1}}{\Gamma(s)} F(t) \frac{dt}{t},$$

where the usual regularization of the logarithm at zero is understood, in which case the integral can be shown to converge on $\Re s > k+1$. In what follows we shall write $L[F](s) := L[F](s, 1)$ and say that the functions $F(z)$ satisfying the conditions given above are k -BIEBERBACH.

This complex iterated integral turns out to coincide under the change of variables $x = -\log t$ with the fractional integral as defined by RIEMANN and LIOUVILLE; for which the *additive iterativity* property

$$(33) \quad L[F](s) = L \left[\int_{[0,z]} F(t) \left(\frac{dt}{t} \right)^w \right] (s - w)$$

holds for those w for which all relevant integrals converge. (w should have $\Re w > k + 1$ and $\Re (s - w) > k + 1$.) Although this much is classical, the iterated integral perspective lends itself to powerful generalization, gives the structure of HOPF algebra on a suitable algebra of formal power series expressions in non-commuting variables (see [Joy]), and has various interesting number theoretic consequences (see [Joy10]), among them the non-classical *multiplicative iterativity* property

$$\int_{[0,1]} \sum_{n=1}^{\infty} a_n z^n \left(\frac{dz}{z} \right)^s = \int_{[0,1]} \sum_{n=1}^{\infty} a_n z^{n^k} \left(\frac{dz}{z} \right)^{s/k}$$

for positive integer k .

Each of these respective iterativity properties gives rise to an infinite family of integral expressions for the RIEMANN zeta function $\zeta(s)$:

Firstly, we remark that integrating along a path from 0 to z in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ against $\frac{dz}{z}$ is essentially inverse to applying the differential operator $z \frac{d}{dz}$. This is the principle idea behind HADAMARD's differo-integration theory (see for example [SKM93]), and finds expression in the following key

Lemma 7.1. *Suppose that $F(z)$ is k -BIEBERBACH. Then*

$$L \left[\left(z \frac{d}{dz} \right)^m F(z) \right] (s + m) = L[F](s) = L \left[\int_{[0,z]} F(z) \left(\frac{dz}{z} \right)^m \right] (s - m)$$

for all $m \in \mathbb{N}$, where the first and second integrals converge provided that $\Re s > k + 1$, while the third integral converges whenever $\Re s > \max\{m, k + 1\}$.

Proof. Firstly note that if $F(z)$ is k -BIEBERBACH, then

$$(34) \quad \left(z \frac{d}{dz} \right)^m F(z) = \sum_{n=1}^{\infty} a_n n^m z^n$$

is $(k + m)$ -BIEBERBACH, (so that the first integral converges), while

$$(35) \quad \int_{[0,1]} F(z) \left(\frac{dz}{z} \right)^m = \sum_{n=1}^{\infty} \frac{a_n}{n^m} z^n$$

is $k - m$ -BIEBERBACH, from which convergence of the third expression in the statement follows.

Now recall (from [Joy10]) that

$$\int_{[0,1]} z^n \left(\frac{dz}{z} \right)^t = \frac{1}{n^t}$$

for $\Re t > 0$, for any $n \geq 1$. This condition on t gives rise to the convergence condition for the third integral.

Then the assertion follows from (34) and (35) once we can justify interchanging the order of integration and summation. But this is a consequence of the LEBESGUE dominated convergence theorem, as a standard argument shows as for example in [Hid93]. \square

Now in the coordinates on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ ABEL's integral for $\zeta(s)$ becomes

$$(36) \quad \zeta(s) = \int_{[0,1]} \frac{z}{1-z} \left(\frac{dz}{z} \right)^s = L \left[\frac{z}{1-z} \right] (s)$$

and hence by the lemma may be expressed by any one of the family of integrals

$$(37) \quad \zeta(s) = \int_{[0,1]} \text{Li}_\mu(z) \left(\frac{dz}{z} \right)^{s-\mu}$$

for integer μ , with $\text{Li}_\mu(z)$ denoting the usual polylogarithm function

$$\text{Li}_\mu(z) := \int_{[0,z]} \frac{t}{1-t} \left(\frac{dt}{t} \right)^\mu$$

when $\mu > 0$, and otherwise the rational function

$$\text{Li}_\mu(z) := \left(z \frac{d}{dz} \right)^\mu \frac{z}{1-z}.$$

On the other hand, by multiplicative iterativity and use of ABEL's integral,

$$\zeta(s) = \int_{[0,1]} \sum_{n=1}^{\infty} z^{n^k} \left(\frac{dz}{z} \right)^{s/k}$$

for positive integer k . Observe that the case of $k = 2$ corresponds to the theta function integral used in RIEMANN's second proof of the functional equation of $\zeta(s)$, under the change of variables $z = e^{-\pi t}$.

Since ABEL's integral (36) (which forms the basis of RIEMANN's first proof of the functional equation) belongs to both families of integrals it is interesting to exhibit a proof of the functional equation making

use of an integral which is a member of the additive family of integrals but not of the multiplicative family. To this we next proceed.

7.3. Analytic continuation at integer parameter $\mu > 1$. Any of the polylogarithm integrals in (37) - barring that with $\mu = 1$ - provides the basis for the analytic continuation of $\zeta(s)$ to all of $\mathbb{C} \setminus \{1\}$. The absence of a proof with parameter 1 is explained by the singularity of $\zeta(s)$ at $s = 1$. More concretely, dealing with positive parameter n , $\zeta(n)$ is a term of the EULER connection formula, or seen otherwise, the DRINFEL'D associator has no linear terms.

In every case, the crucial ideas in the analytic continuation are the same:

For example, considering the dilogarithm integral

$$\zeta(s) = \int_{[0,1]} \text{Li}_2(z) \left(\frac{dz}{z} \right)^{s-2} = \int_0^\infty \text{Li}_2(e^{-x}) \frac{x^{s-2}}{\Gamma(s-2)} \frac{dx}{x},$$

(where we take $x = -\log z$ to obtain the last integral), for the analytic continuation of this integral to complex values of s for which $\Re s \leq 2$ the standard (HANKEL) contour C slightly above the real axis beginning at $+\infty$, encircling 0 in the positive direction and returning to $+\infty$ slightly below the real axis is not suitable, because the dilogarithm monodromy term arising from moving about 0 is $2\pi i x$, which does not have finite MELLIN transform. Instead we borrow an idea from the sine transform proof of the functional equation for $\zeta(s)$ due to TITCHMARSH (see [Tit30]), to deal with the singularity at $x = 0$ and hence achieve the analytic continuation to $1 < \Re s < 2$. The resulting integral lends itself nicely to the use of EULER'S dilogarithm inversion formula, which is a functional equation of the dilogarithm effecting a change between $z = 0$ and $z = 1$. This effectively shifts the monodromy of $\text{Li}_2(e^{-x})$ to $x = +\infty$, so that HANKEL'S contour may be used.

Now write $\text{Li}_{2,1 \times (n-2)}(z) := \text{Li}_{211\dots 1}(z)$ with the index 1 repeated $n - 2$ times; i.e. the multiple polylogarithm

$$\text{Li}_{211\dots 1}(z) = \int_{[0,z]} \frac{dz}{1-z} \frac{dz}{z} \frac{dz}{1-z} \frac{dz}{1-z} \cdots \frac{dz}{1-z}$$

in which the form $\frac{dz}{1-z}$ occurs a total of $n - 1$ times. In general we find

Theorem 7.2. *For each integer $m \geq 2$,*

$$\zeta(s) = -\frac{(s-m)\Gamma(m)\Gamma(1-s)}{2\pi i} \int_C \frac{\text{Li}_{2,1 \times (m-2)}(1-e^{-x})}{x^m} (-x)^s \frac{dx}{x}$$

for all complex $s \neq 1$ satisfying $\Re s < m$.

For each fixed m , together with (37) this result gives the analytic continuation of $\zeta(s)$ to all values other than $\{1\} \cup \{\Re s = m\}$.

Notice that the proof makes essential use of the EULER connection formula encoded in (4) - i.e. 4.7 in addition to the monodromy data of 4.10.

Proof. Throughout let m denote an integer with $m \geq 2$. Then

$$\begin{aligned} \zeta(s) &= \int_0^1 \text{Li}_m(e^{-x}) \frac{x^{s-m}}{\Gamma(s-m)} \frac{dx}{x} + \int_1^\infty \text{Li}_m(e^{-x}) \frac{x^{s-m}}{\Gamma(s-m)} \frac{dx}{x} \\ &= \int_0^1 \left[\frac{\text{Li}_m(e^{-x})}{x} - \frac{\zeta(m)}{x} \right] \frac{x^{s-m}}{\Gamma(s-m)} dx + \frac{\zeta(m)}{s-m} + \int_1^\infty \text{Li}_m(e^{-x}) \frac{x^{s-m}}{\Gamma(s-m)} \frac{dx}{x}. \end{aligned}$$

This last expression holds also for $m-1 < \Re s < m$ by analytic continuation, since $\text{Li}_m(e^0) = \zeta(m)$. But on this vertical strip,

$$\frac{1}{s-m} = - \int_1^\infty x^{s-m-1} dx.$$

Consequently, provided that $m-1 < \Re s < m$, we can write

$$(38) \quad \zeta(s) = \int_0^\infty \left(\frac{\text{Li}_m(e^{-x}) - \zeta(m)}{x} \right) \frac{x^{s-m}}{\Gamma(s-m)} dx.$$

(This much is borrowed from a similar analytic continuation in [Tit30].)

Now from [OU05] using exponential coordinates and $\text{Li}_1(z) = -\log(1-z)$, EULER'S connection formula takes the form of

$$\begin{aligned} \text{Li}_m(e^{-x}) - \zeta(m) &= -\text{Li}_{2,1 \times (m-2)}(1-e^{-x}) - \frac{x^{m-1}}{(m-1)!} (-\log(1-e^{-x})) \\ &\quad - \frac{x^{m-2}}{(m-2)!} \text{Li}_2(e^{-x}) - \dots - \frac{x^2}{2!} \text{Li}_{m-2}(e^{-x}) - x \text{Li}_{m-1}(e^{-x}). \end{aligned}$$

In substituting this expression into (38) we notice immediately that all other polylogarithm integral expressions as in (37) with $\mu = 1, \dots, m-1$ appear. These expressions are also valid for $m-1 < \Re s < m$, so in each case, the resulting expression may be replaced by some multiple of $\zeta(s)$. We show this explicitly when $m = 2$: Then,

$$(39) \quad \zeta(s) = \int_0^\infty \left(\frac{\log(1-e^{-x})}{x} - \frac{\text{Li}_2(1-e^{-x})}{x^2} \right) \frac{x^{s-1}}{\Gamma(s-2)} dx$$

whenever $1 < \Re s < 2$. Here, for $\Re s > 1$ we have

$$\zeta(s) = \int_{[0,1]} \text{Li}_1(z) \left(\frac{dz}{z} \right)^{s-1} = - \int_0^\infty \log(1-e^{-x}) \frac{x^{s-1}}{\Gamma(s-1)} \frac{dx}{x}.$$

From $(s-2)\Gamma(s-2) = \Gamma(s-1)$ it then follows that

$$(40) \quad \int_0^\infty \frac{\log(1-e^{-x})}{x} \frac{x^{s-1}}{\Gamma(s-2)} dx = -(s-2)\zeta(s),$$

for $1 < \Re s < 2$. Then using (40) in (39),

$$(s-1)\zeta(s) = - \int_0^\infty \frac{\text{Li}_2(1-e^{-x})}{x^2} \frac{x^{s-1}}{\Gamma(s-2)} dx.$$

Most generally, repeated use of the functional equation

$$(41) \quad \Gamma(r+1) = r\Gamma(r)$$

together with (37) shows that for each integer k with $1 \leq k \leq m-1$,

$$\begin{aligned} - \int_0^\infty \frac{x^{m-k} \text{Li}_k(e^{-x})}{(m-k)!x} \frac{x^{s-m}}{\Gamma(s-m)} dx &= - \frac{(s-m) \dots (s-k-1)}{(m-k)!} \zeta(s) \\ &= - \binom{s-k-1}{m-k} \zeta(s). \end{aligned}$$

Adding the negative of such expressions to both sides of our equation for $\zeta(s)$ (found by substitution of the EULER connection formula into (38)) and using a simple inductive argument to add up the terms of the coefficient, (adding first $1 + (s-m)$ to obtain $s-m+1$ then taking this as a common factor in summing with the next term and so on), the left side becomes

$$\left[1 + \binom{s-m}{1} + \dots + \binom{s-2}{m-1} \right] \zeta(s) = \binom{s-1}{m-1} \zeta(s)$$

while the right side is given by

$$- \int_0^\infty \text{Li}_{2,1 \times (m-2)}(1-e^{-x}) \frac{x^{s-m}}{\Gamma(s-m)} \frac{dx}{x}.$$

By equating coefficients of the first equation of 4.10, one sees that $\text{Li}_{2,1 \times (m-2)}(z)$ has no monodromy about $z = 0$. Thus, $\text{Li}_{2,1 \times (m-2)}(1-e^{-x})$ has no monodromy about $x = 0$. Now with C as above, consider

$$I(s) := \int_C \frac{\text{Li}_{2,1 \times (m-2)}(1-e^{-x})}{x^m} (-x)^{s-1} dx.$$

Here the branch cut for the logarithm is taken along the negative real axis, so that for the portion of C above the real axis from $x = +\infty$ to $x = 0$,

$$(-x)^s = e^{s(\log x - i\pi)}$$

and along the part of C below the real axis back from 0 to $+\infty$,

$$(-x)^s = e^{(s \log x + i\pi)}.$$

Now along the circle, say $|x| = \varepsilon$, which is the piece of C around $x = 0$, the integrand is bounded by

$$M\varepsilon |x^{(\Re s)-m}| e^{2\pi\varepsilon}$$

for some constant $M > 0$ because $\text{Li}_{2,1 \times (m-2)}(1 - e^{-x})$ vanishes at $x = 0$ at least to the same order as does x . Now since $\Re s > m - 1$, the integral about $|x| = \varepsilon$ approaches 0 as ε becomes very small. (The integral goes on the order of $\varepsilon^{\Re s - m + 1}$.)

Consequently, in the limit as ε approaches 0, we have

$$\begin{aligned} I(s) &\rightarrow -e^{-i\pi s} \int_{\infty}^0 \frac{\text{Li}_{2,1 \times (m-2)}(1 - e^{-x})}{x^m} x^s \frac{dx}{x} \\ &\quad - e^{i\pi s} \int_0^{\infty} \frac{\text{Li}_{2,1 \times (m-2)}(1 - e^{-x})}{x^m} x^s \frac{dx}{x} \\ &= (e^{i\pi s} - e^{-i\pi s}) \binom{s-1}{m-1} \Gamma(s-m) \zeta(s). \end{aligned}$$

Now $2i \sin(\pi s) = e^{i\pi s} - e^{-i\pi s}$ and we may repeatedly use (41) to see that

$$\binom{s-1}{m-1} \Gamma(s-m) = \frac{\Gamma(s)}{(s-m) \cdot (m-1)!} = \frac{\Gamma(s)}{(s-m)\Gamma(m)}.$$

Moreover,

$$\frac{\pi}{\sin \pi s} = \Gamma(s)\Gamma(1-s),$$

so that

$$\begin{aligned} (e^{i\pi s} - e^{-i\pi s}) \binom{s-1}{m-1} \Gamma(s-m) &= 2i \sin(\pi s) \frac{\Gamma(s)}{(s-m)\Gamma(m)} \\ &= \frac{2i\pi}{(s-m)\Gamma(m)\Gamma(1-s)}. \end{aligned}$$

Hence

$$(42) \quad \zeta(s) = \frac{(s-m)\Gamma(m)\Gamma(1-s)}{2\pi i} \int_C \frac{\text{Li}_{2,1 \times (m-2)}(1 - e^{-x})}{x^m} (-x)^{s-1} dx.$$

This expression has been proven for $m > \Re s > m - 1$, but converges for all s having $\Re s < m$ with the possible exception of the poles $s = 1, \dots, m-1$ of $\Gamma(1-s)$ in this region of the plane. (When $\Re s \geq m$, the integrand exhibits unsuitable behavior at infinity.) However, for $s = 2, \dots, m-1$ the integral vanishes by CAUCHY'S Theorem, since along the real axis, L'HÔPITAL'S Rule shows that

$$\lim_{x \rightarrow 0} \frac{\text{Li}_{2,1 \times (m-2)}(1 - e^{-x})}{x^{m-1}} = \frac{1}{(m-1)!(m-1)}$$

where the derivative of $\text{Li}_{2,1 \times (m-2)}(1 - e^{-x})$ is

$$\frac{e^{-x}}{1 - e^{-x}} \frac{x^{m-1}}{(m-1)!}.$$

This leaves only the simple pole at $s = 1$, for which we may compute the residue as usual: Firstly,

$$\text{Res}_{s=1} \Gamma(1-s) = -1,$$

so

$$\begin{aligned} \text{Res}_{s=1} \zeta(s) &= \lim_{s \rightarrow 1} (s-1) \Gamma(1-s) \frac{2\pi i}{(m-1)!(m-1)} \frac{(s-m)\Gamma(m)}{2\pi i} \\ &= (-1) \frac{(1-m)(m-1)!}{(m-1)!(m-1)} = 1 \end{aligned}$$

as is well known.

The analytic continuation for $\zeta(s)$ to $\Re s < m$ is achieved by (42). \square

7.4. Dilogarithm proof of the functional equation. Lifting the analytic continuation integral (42) to the RIEMANN surface on which the logarithm function is single valued, and computing by means of CAUCHY'S Theorem, the functional equation of $\zeta(s)$ may be proven. In principle, this may be done for each value of $m \geq 2$ using the monodromy of $\text{Li}_{2,1 \times (m-2)}(z)$ as may be calculated using 4.10 and the ideas of [MPvdH00]. (In the notation of that paper, $\text{Li}_{2,1 \times (m-2)}(z) = L_{x_1^{m-2} x_0 x_1}(z)$.)

The interesting aspect of the computation is that the monodromy terms coming from considering $\text{Li}_{2,1 \times (m-2)}(1 - e^{-x})$ around ∞ have themselves monodromy about the lifts of 1 (namely at $2\pi i n$ for integer n), and this monodromy of the monodromy is what contributes terms that add up to $\zeta(1-s)$ multiplied by some factor.

All such proofs follow the same pattern, so for clarity of exposition, we restrict ourselves to the case that $m = 2$ and present a careful proof in this situation:

Consider a copy of \mathbb{C} which should really be thought of as the punctured surface $X_{\log} \xrightarrow{\sim} \mathbb{C} \setminus 2\pi i \mathbb{Z}$ on which the logarithm function is single valued, but which we shall consider as merely having a logarithmic branch cut along the negative real axis. Let $a \rightarrow b$ denote the straight line segment from a to b in \mathbb{C} . Then let $C_{R,N}$ denote the following succession of paths: Firstly, a loop C_0 about 0 from some large $R \gg 0$ and back - more precisely a path beginning with $R - i\varepsilon \rightarrow \delta - i\varepsilon$ then looping about 0 in the negative direction to a point $\delta + i\varepsilon$ followed by the

straight line segment ending at $R + i\varepsilon$, where ε and δ are small positive real numbers; next $R + i\varepsilon \rightarrow R + 2\pi i - i\varepsilon$ proceeding with $C_0 + 2\pi i$ and thereafter a line segment to $R + 4\pi i - i\varepsilon$ preceeding $C_0 + 4\pi i$; and on in this way to some $C_0 + 2N\pi i$ for some large $N \in \mathbb{N}$. Next, a line segment to $R + (2N + 1)\pi i$ followed by $R + (2N + 1)\pi i \rightarrow -R + (2N + 1)\pi i \rightarrow -R - (2N + 1)\pi i \rightarrow R - (2N + 1)\pi i \rightarrow R - 2N\pi i - i\varepsilon$. Subsequently, $C_0 - 2N\pi i$ followed by the path which is the mirror image about the real axis of that described above, until reaching the starting point $R - i\varepsilon$.

Now $\text{Li}_2(1 - e^{-x})$ has the monodromy terms $2\pi i \log(1 - e^{-x})$ along the paths $R + 2k\pi i \rightarrow R + 2(k + 1)\pi i$ (for integer k), since $\text{Li}_2(z)$ has monodromy term $-2\pi i \log z$ moving in a positive direction around $z = 1$; and as x rises by $2\pi i$ in \mathbb{C} , $1 - e^{-x}$ describes a negatively oriented circle about $x = 1$. These logarithmic terms themselves have monodromy of $2\pi i$ about $2k\pi i$ for integer k , because $1 - e^{-x} = 0$ at such points, and for η sufficiently small, a negatively oriented loop of radius η about $2k\pi i$ maps to a positively oriented path encircling $x = 0$ under $x \mapsto 1 - e^{-x}$.

Hence, the region enclosed by such a path $C_{R,N}$ contains none of the points at which the integrand (42) nor the monodromy terms are singular, for $\Re s < 0$. By CAUCHY'S Theorem then,

$$\frac{(s - 2)\Gamma(1 - s)}{2\pi i} \int_{C_{R,N}} \frac{\text{Li}_2(1 - e^{-x})}{x^2} (-x)^s \frac{dx}{x} = 0.$$

We proceed to compute this integral, under the assumption that $\Re s < -2$.

Firstly, we know that in the limit as ε and δ approach 0 and R nears ∞ , the integral along C_0 tends to $-\zeta(s)$. Next we have

$$\frac{(s - 2)\Gamma(1 - s)}{2\pi i} \int_{R+i\varepsilon}^{R+2\pi i-i\varepsilon} \frac{\text{Li}_2(1 - e^{-x})}{x^2} (-x)^s \frac{dx}{x},$$

but passage along this line segment produces a monodromy term from the dilogarithm, of

$$(43) \quad \frac{2\pi i \log(1 - e^{-x})}{x^3} (-x)^s$$

which must be taken into account along all subsequent paths.

Now the dilogarithm integral along the translate $C_0 + 2\pi i$ approaches 0 as ε tends to 0 by CAUCHY'S Theorem. In particular, notice that $(-x)^s$ has the same value on the straight line segments of this part of the path, so that the integral of the monodromy term involving $\log(1 - e^{-x})$ also vanishes along these straight line segments. What remains to consider

then from this portion of $C_{R,N}$ is

$$\frac{(s-2)\Gamma(1-s)}{2\pi i} \int_{\gamma_1} \frac{2\pi i \log(1-e^{-x})}{x^2} (-x)^s \frac{dx}{x}$$

where γ_k will denote the (negatively oriented) loop about $2\pi i k$ for integer k , along with

$$(s-2)\Gamma(1-s)(2\pi i) \int_{2\pi i+\delta+i\varepsilon}^{R+2\pi i+i\varepsilon} (-x)^{s-2} \frac{dx}{x},$$

the term arising from the monodromy of $\log(1-e^{-x})$ about $2\pi i$. As before, this last integrand must be considered along all subsequent subpaths of $C_{R,N}$. But notice that along the remaining translates of C_0 , this monodromy term (from passage around $2\pi i$) is 0 (again in the limit as $\varepsilon \rightarrow 0$) by CAUCHY'S Theorem.

Now let $D_{R,n}$ denote the rectangular path $R+2n\pi i \rightarrow R+(2N+1)\pi i \rightarrow -R+(2N+1)\pi i \rightarrow -R-(2N+1)\pi i \rightarrow R-(2N+1)\pi i \rightarrow R-2n\pi i$ for non-negative integer $n \leq N$. Continuing along $C_{R,N}$ we find thus that the integrals which are yet to be computed add to

$$\begin{aligned} & \frac{(s-2)\Gamma(1-s)}{2\pi i} \int_{D_{R,0}} \frac{\text{Li}_2(1-e^{-x})}{x^2} (-x)^s \frac{dx}{x} \\ & + \sum_{n=1}^N \frac{(s-2)\Gamma(1-s)}{2\pi i} \int_{\gamma_n} \frac{n 2\pi i \log(1-e^{-x})}{x^2} (-x)^s \frac{dx}{x} \\ & + \frac{(s-2)\Gamma(1-s)}{2\pi i} \sum_{n=1}^N \left\{ \int_{2n\pi i+\delta+i\varepsilon}^{R+2n\pi i+i\varepsilon} n(2\pi i)^2 (-x)^{s-2} \frac{dx}{x} \right. \\ & \left. + \int_{D_{R,n}} \sum_{m=1}^n m(2\pi i)^2 (-x)^{s-2} \frac{dx}{x} \right\} \end{aligned}$$

along with terms with integrand of the form of (43) integrated along the outside contour.

Now along the portion of $C_{R,N}$ proceeding from the point $-R+(2N+1)\pi i$, further monodromy terms arise from the dilogarithm terms, in this instance the negatives of terms of the form of (43). All such terms themselves exhibit monodromy each time the path traverses a segment of length $2\pi i$ along the line $-R+2N\pi i \rightarrow -R-2N\pi i$ since images of such segments trace out circles of radius e^R about $z=1$ under the mapping $x \mapsto 1-e^{-x}=z$.

These new dilogarithm monodromy terms cancel out those from the first vertical portion of the path, so that all such terms add to zero by

when the point $-R$ is reached along $C_{R,N}$. Below the real axis, negative terms accumulate so that once one reaches the point $-R - (2N+1)\pi i$, the remaining dilogarithm monodromy terms add to

$$-2\pi i N \log(1 - e^{-x}).$$

On the other hand, since the number of logarithmic terms as one moves along $-R + i\alpha$ (for real decreasing α) decreases from N to $N-1$ to $N-2$ and so on, the sum of the logarithmic monodromy terms number successively $N(N+1)/2$; $N(N+1)/2 + N$; then $N(N+1)/2 + N + (N-1)$ and so on, until at the point $-R$, there are $N(N+1)$ such terms. Thereafter, the increasing number of negative logarithmic terms decrease the total number of these second monodromy terms. Eventually, at $-R - (2N+1)\pi i$, the end of the vertical line, the terms which remain sum to

$$(2\pi i)^2 [1 + 2 + \dots + N].$$

By the same argument as before, the integral coming from the terms $(2\pi i)^2 [1 + 2 + \dots + N - 1]$ is zero around $C_0 - 2N\pi i$, but because of the monodromy of the log term about $-2N\pi i$, the integral

$$\frac{(s-2)\Gamma(1-s)}{2\pi i} \int_{R-2N\pi i-i\varepsilon}^{-2N\pi i+\delta-i\varepsilon} N(2\pi i)^2 (-x)^{s-2} \frac{dx}{x}$$

does need to be taken into account. Continuing back to the starting point of $C_{R,N}$, similar terms add to

$$\frac{(s-2)\Gamma(1-s)}{2\pi i} \sum_{n=1}^N \int_{R-2n\pi i-i\varepsilon}^{-2n\pi i+\delta-i\varepsilon} n(2\pi i)^2 (-x)^{s-2} \frac{dx}{x}.$$

This expression, along with its counterpart from the part of $C_{R,N}$ with positive imaginary part, is readily computed in the limit that δ and ε approach 0 while R tends to ∞ : Indeed, by using CAUCHY'S Theorem applied to rectangular contours respectively below and above the real axis, we find that

$$(44) \quad \lim_{R \rightarrow \infty; \delta, \varepsilon \rightarrow 0} \int_{R-2n\pi i-i\varepsilon}^{-2n\pi i+\delta-i\varepsilon} n(2\pi i)^2 (-x)^{s-2} \frac{dx}{x} = \frac{(2\pi)^s (i)^s n^{s-1}}{s-2}$$

whereas

$$(45) \quad \lim_{R \rightarrow \infty; \delta, \varepsilon \rightarrow 0} \int_{2n\pi i+\delta+i\varepsilon}^{R+2n\pi i+i\varepsilon} n(2\pi i)^2 (-x)^{s-2} \frac{dx}{x} = -\frac{(2\pi)^s (-i)^s n^{s-1}}{s-2}.$$

More precisely, taking $\varepsilon\delta \rightarrow 0$, consider the contour $E_{R,n,\kappa,-}$ formed by

$$R - 2\pi i n \rightarrow -2\pi i n \rightarrow -i\kappa \rightarrow R - i\kappa \rightarrow R - 2\pi i n$$

where $\kappa > 0$ is small. Then one computes

$$\int_{-2\pi i n}^{-i\kappa} \frac{(-x)^s}{x^2} \frac{dx}{x} = e^{i\frac{\pi}{2}s} \frac{(2\pi n)^{s-2}}{s-2} - e^{i\frac{\pi}{2}s} \frac{\kappa^{s-2}}{s-2}$$

and

$$\int_{-i\kappa}^{R-i\kappa} \frac{(-x)^s}{x^2} \frac{dx}{x} = e^{i\pi s} \frac{(R-i\kappa)^{s-2}}{s-2} + e^{i\frac{\pi}{2}s} \frac{\kappa^{s-2}}{s-2}.$$

while

$$\left| \int_{R-i\kappa}^{R-2\pi i n} \frac{(-x)^s}{x^2} \frac{dx}{x} \right| \leq K_E 2\pi \cdot \max \left\{ \left| \frac{(-x)^s}{x^2} \right| \right\}$$

where $K_E > 0$ is constant and the maximum is taken over the straight line segment $R - i\kappa \rightarrow R - 2\pi i n$, so that this last integral approaches zero as R grows without bound. Adding these integrals in the limit that $R \rightarrow \infty$, we obtain

$$(-i^{-2})i^s \frac{(2\pi n)^{s-2}}{s-2}$$

and by CAUCHY'S Theorem, the integral in (44) is the negative of this quantity multiplied by $n(2\pi i)^2$, from which we deduce the equality in (44). A similar computation suffices to show the validity of (45).

Adding all such terms of the integral along $C_{R,N}$ then gives

$$\begin{aligned} & \frac{(s-2)\Gamma(1-s)}{2\pi i} \frac{(2\pi)^s [i^s - (-i)^s]}{s-2} \sum_{n=1}^{\infty} n^{s-1} \\ &= \Gamma(1-s) 2^s \pi^{s-1} \frac{e^{i\frac{\pi}{2}s} - e^{-i\frac{\pi}{2}s}}{2i} \zeta(1-s) \\ &= \Gamma(1-s) 2^s \pi^{s-1} \sin\left(\frac{\pi s}{2}\right) \zeta(1-s). \end{aligned}$$

Since this term added to $-\zeta(s)$ gives 0, the functional equation follows.

It remains to be shown that in the limit, the remaining terms approach 0. It is convenient to assume that $2(2N+1)\pi < R$

We begin with the integral

$$(46) \quad \int_{D_{R,0}} \frac{\text{Li}_2(1-e^x)}{x^2} (-x)^s \frac{dx}{x}$$

where the monodromy terms are ignored. This is most readily approximated by considering separately the two portions of the path $D_{R,0}$ on respective sides of the imaginary axis, say $D_{R,+}$ for the part with non-negative real part and its counterpart $D_{R,-}$ to the left of the imaginary axis.

Now both $D_{R,+}$ and $D_{R,-}$ have length $2R + 2(2N + 1)\pi < 3R$ by the assumption on N .

Along $D_{R,+}$, $|\text{Li}_2(1 - e^{-x})| \leq (\zeta(2) + \text{Li}_2(2)\varepsilon_R)$ where $\varepsilon > 0$ approaches 0 as $R \rightarrow \infty$ since $1 - e^{-x}$ is close to 0 along $R + i\alpha$ for real α , while $\text{Li}_2(1 - e^{-x}) = \text{Li}_2(1 + e^{-l})$ for positive l along both $R + (2N + 1)\pi i \rightarrow (2N + 1)\pi i$ and $-(2N + 1)\pi i \rightarrow R - (2N + 1)\pi i$. Because the points of $D_{R,+}$ are outside of a circle of radius R , also

$$\left| \frac{(-x)^s}{x^3} \right| = |x|^{\Re s - 3} \leq R^{\Re s - 3}.$$

Hence, for C and C' denoting positive constants, a bound on the absolute value of the part of (46) along $D_{R,+}$ is

$$CR^{\Re s - 2}(\zeta(2) + \text{Li}_2(2) + \varepsilon_R)(2R + 2(2N + 1)\pi) < C'R^{\Re s - 1} \rightarrow 0$$

as R tends to ∞ , because $\Re s < -2$.

Now on $D_{R,-}$ we again use EULER inversion to rewrite the integral as

$$(47) \quad \int_{D_{R,-}} [\zeta(2) - \text{Li}_2(e^{-x}) + x \log(1 - e^{-x})] \frac{(-x)^s}{x^2} \frac{dx}{x}.$$

Now $\text{Li}_2(e^{-x}) + \zeta(2)$ may be bounded along $D_{R,-}$ in similar vein to the bound obtained for $\text{Li}_2(1 - e^{-x})$ along $D_{R,+}$ and it hence follows that the contribution from these first two terms approaches zero as $R \rightarrow \infty$. As for the logarithmic term, notice that for $x \in \mathbb{R}$,

$$\lim_{x \rightarrow -\infty} \frac{\log(1 - e^{-x})}{x^2} = 0$$

by L'HÔPITAL'S Rule. Consequently, for any given $\eta > 0$, one may choose R sufficiently large so that also

$$(48) \quad \left| \frac{\log(1 - e^{-x})}{x^2} \right| < \eta$$

for any x on $D_{R,-}$. Thence, a bound on the third term of (47) is

$$K\eta R^{\Re s + 1}(2R + 2(2N + 1)\pi) < K'\eta R^{\Re s + 2}$$

(with positive constants K and K'), which tends to 0 as R goes to infinity, since we assume that $\Re s < -2$.

These estimates also serve to deal with the logarithmic terms coming from the monodromy of the dilogarithm, integrated along the boundary. In particular, it is easily seen that the bound (48) holds along all of $D_{R,0}$ if η is chosen suitably. Now the absolute value of the number

of such logarithmic terms is at most N , so if K'' and K''' denote some positive constants, the sum of such integrals is bounded above by

$$\begin{aligned} N \left| \int_{D_{R,0}} \frac{\log(1 - e^{-x})}{x^2} (-x)^s \frac{dx}{x} \right| &< K'' N \eta R^{\Re s} (4R + 4(2N + 1)\pi) \\ &< K''' \eta R^{\Re s + 2} \end{aligned}$$

which as before can be made arbitrarily small.

Next consider the integrals

$$\sum_{n=1}^N \int_{\gamma_n} \frac{n 2\pi i \log(1 - e^{-x})}{x^2} (-x)^s \frac{dx}{x}.$$

For each n , make the change of variables $y = x - 2\pi i n$ to obtain

$$\begin{aligned} &\sum_{n=1}^N \int_{\gamma_0} \frac{n 2\pi i \log(1 - e^{-y})}{(y + 2\pi i n)^3} (-y - 2\pi i n)^s dy \\ &= \sum_{n=1}^N \int_{\gamma_0} \frac{n 2\pi i y \log(1 - e^{-y})}{(y + 2\pi i n)^3} (-y - 2\pi i n)^s \frac{dy}{y}. \end{aligned}$$

Along the real axis, L'HÔPITAL'S Rule gives

$$\lim_{y \rightarrow 0} y \log(1 - e^{-y}) = 0,$$

so that any point z along γ_0 has

$$|z \log(1 - e^{-z})| \leq |y_0(\log(1 - e^{-y_0}) + 2\pi i)| < \eta'$$

where y_0 lies on $\gamma_0 \cap \mathbb{R}_{>0}$ and $\eta' > 0$ approaches 0 with δ . This shows that

$$\begin{aligned} &\left| \int_{\gamma_0} y \log(1 - e^{-y}) \frac{(-y - 2\pi i n)^s}{(y + 2\pi i n)^3} \frac{dy}{y} \right| \\ &\leq \eta' \left| \int_{\gamma_0} \frac{(-y - 2\pi i n)^s}{(y + 2\pi i n)^3} \frac{dy}{y} \right| \\ &= \eta' (2\pi n)^{\Re s - 3} \end{aligned}$$

using the calculus of residues for the last computation. Adding now all such terms along with the similar integrals along loops around $-2\pi i n$ for $n \geq 0$, the bound computes to $\eta' 2(2\pi)^{\Re s - 3} \zeta(2 - s)$ and this evidently tends to 0 as η' does.

Finally we dispense with the terms arising from monodromy of the logarithmic terms, integrated along the outside of the contour. The

largest number of such terms at any point along the contour is $N(N+1)$ so that the sum of all such integrals is certainly bounded by

$$N(N+1)(4R+4(2N+1)\pi)R^{\Re s-2} < R^{\Re s+1}$$

which becomes arbitrarily small as R grows without bound.

REFERENCES

- [Car01] P. Cartier. Fonctions polylogarithmes, nombres polyzêtas et groupes pro-unipotents. *Sém. Bourbaki*, exp. n° 885, 2000-2001.
- [Cha80] K. Chandrasekharan. *Elliptic functions*. Springer-Verlag, 1980.
- [Del70] P. Deligne. Equations différentielles à points singuliers réguliers. Number 163 in *Lecture notes in mathematics*. Springer-Verlag, 1970.
- [Del89] P. Deligne. Le groupe fondamental de la droite projective moins trois points. In *Galois Groups over \mathbb{Q}* , pages 79–297. Springer-Verlag, 1989.
- [Dri91] V.G. Drinfel’d. On quasitriangular quasi-hopf algebras and a group closely connected with $\text{Gal}(\mathbb{Q}/\mathbb{Q})$. *Leningrad Math J.*, 2(4):829–860, 1991.
- [Hai] R. Hain. *Lectures on the Hodge-De Rham Theory of $\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\})$* . Arizona Winter School 2003.
- [Hai94] R. Hain. Classical polylogarithms. In *Motives (Seattle, WA, 1991)*, volume 55 of *Proc. Sympos. Pure Math.*, pages 3–42. Amer. Math. Soc., 1994.
- [Hai03] R. Hain. Periods of limit mixed hodge structures. *Current developments in mathematics*, pages 113–133, 2003.
- [Hec36] E. Hecke. Über die bestimmung dirichletscher reihen durch ihre funktionalgleichung. *Math. Ann.*, 112:664–699, 1936.
- [Hid93] H. Hida. *Elementary theory of L -functions and EISENSTEIN series*. Number 26 in *LMS Student Texts*. Cambridge University Press, 1993.
- [Joy] S.T. Joyner. *The generalized HOPF algebra of complex iterated integrals*. In preparation.
- [Joy08] S.T. Joyner. Zeta functions as iterated integrals. Ph.D. Thesis, Purdue University, 2008.
- [Joy10] S.T. Joyner. On a generalization of CHEN’S iterated integrals. *J. Number Theory*, 130(2):254–288, 2010.
- [Kim09] M. Kim. The unipotent ALBANESE map and SELMER varieties for curves. *Publ. Res. Inst. Math. Sci.*, 45(1):89–133, 2009.
- [Lan85] S. Lang. *$SL_2(R)$* , volume 105 of *Graduate texts in mathematics*. Springer-Verlag, 1985.
- [LM96] T.Q.T. Le and J. Murakami. KONTSEVICH’S integral for the KAUFFMAN polynomial. *Nagoya Math. J.*, 142:39–65, 1996.
- [MPvdH00] H. N. Minh, M. Petitot, and J. van der Hoeven. Shuffle algebra and polylogarithms. *Discrete Mathematics*, 225:217–230, 2000.
- [OU05] J. Okuda and K. Ueno. The sum formula of multiple zeta values and connection problem of the formal KNIZHNIK-ZAMOLODCHIKOV equation. In *Zeta functions, topology and quantum physics*, volume 14 of *Dev. Math.*, pages 145–170. Springer, 2005.

- [Reu93] Reutenauer. *Free LIE groups*. Number New series 7 in LMS Monographs. Oxford University Press, 1993.
- [Rie92] B. Riemann. Ueber die anzahl der primzahlen unter einer gegebenen grosse. In *Gesammelte Werke*. Teubner, 1892.
- [SKM93] S.G. Samko, A.A. Kilbas, and O.I. Marichev. *Fractional integrals and derivatives: theory and applications*. Gordon and Breach Science Publishers, 1993.
- [Tit30] E.C. Titchmarsh. *The theory of the RIEMANN zeta function*. Oxford University Press, 1930.

Sheldon T Joyner, Mathematics Department, The University of Western Ontario, Middlesex College, London, Ontario N6A 5B7, Canada
email: `sjoyner@uwo.ca`